

CURRICULUM VITAE NAZZARENO RE

1. Informazioni personali

Nato ad Ascoli Piceno (AP) il 5.9.1960.

Residente a Pescara (PE) in Via M. Mantini 7, 65125.

Lingue parlate: Italiano (lingua madre), Inglese (fluente), Francese (fluente)

2. Istruzione e formazione

1978: Diploma Liceo Scientifico B. Rossetti di San Benedetto del Tronto (AP).

1978-1983: Corso di laurea in Chimica all'Università degli Studi di Perugia.

1983: Laurea in Chimica all'Università degli Studi di Perugia con il voto 110/110 e lode, discutendo una tesi dal titolo "Teorie Semiclassiche in Cinetica Chimica".

1986-1989: Corso triennale di Perfezionamento in Chimica presso la Scuola Normale Superiore di Pisa (equipollente al Dottorato di Ricerca), lavorando su una tesi dal titolo "Theoretical study of some tetradentate Schiff bases complexes of cobalt".

Novembre 1990 - aprile 1993: Borsa di studio dell'IBM presso il Dipartimento di Chimica dell'Università di Perugia, svolgendo ricerche sull'applicazione di metodi computazionali avanzati allo studio teorico di sistemi molecolari complessi.

Maggio 1993 - luglio 1994: Borsa di studio del CNR presso i laboratori del Prof. C. Floriani dell'Università di Losanna (Svizzera) per svolgere ricerche sull'interpretazione teorica del comportamento magnetico di molecole organometalliche.

3. Esperienze professionali

Novembre 1985- aprile 1986: Azienda Farmaceutica Bristol Europe SpA, Latina (LT) come chimico nel Laboratorio di Ricerca e Sviluppo.

Aprile 1989- ottobre 1990: Enichem, San Donato Milanese (MI) nei Laboratori Materiali Funzionali come responsabile di ricerche sullo sviluppo di materiali sol-gel multielemento.

Agosto 1994 – ottobre 1998: Ricercatore Universitario Università degli Studi di Perugia.

Novembre 1998 – settembre 2002: Professore II Fascia Università degli Studi "G. d'Annunzio" Chieti-Pescara

Ottobre 2002 – presente: Professore I Fascia Università degli Studi "G. d'Annunzio" Chieti-Pescara

4. Capacità e competenze nell'ambito della gestione e valutazione universitaria

2005-2006 Coordinatore scientifico nazionale del Progetto di Rilevante Interesse Nazionale (PRIN) 2004: Fattori stereodinamici che regolano la formazione e le proprietà dei microaggregati. Unità locali coordinate delle Università di Roma Sapienza, Perugia, Palermo, Brescia, Camerino e Chieti.

2007-2008 Coordinatore scientifico nazionale del Progetto di Rilevante Interesse Nazionale (PRIN) 2006: Dalle singole molecole a complessi e nanoaggregati: struttura, chiralità, reattività e teoria. Unità locali coordinate delle Università di Roma Sapienza, Perugia, Potenza e Chieti.

2010-2012: Coordinatore scientifico nazionale del Progetto di Rilevante Interesse Nazionale (PRIN) 2009: Fotoni, radicali e molecole cariche coinvolti in sistemi di interesse nelle bio e nanotecnologie. Unità locali coordinate delle Università di Roma Sapienza, Perugia, Potenza e Chieti.

2009-2011: Presidente del Consiglio di Corso di Laurea in Farmacia per gli a.a 2009/2010 e 2010/2011.

2011-2013: Presidente del Consiglio di Corso di Laurea in Chimica e Tecnologia Farmaceutiche (CTF) per gli a.a 2011/2012 e 2012/2013.

2010-presente : Coordinatore di Facoltà/Dipartimento del progetto LLP Erasmus.

2009-2012 : Membro del Consiglio di Amministrazione dell'Ateneo G. D'Annunzio, Chieti.

2011-2012 : Presidente della Commissione Appalti di Ateneo del CdA.

2013-2015 : Presidente del Nucleo di Valutazione dell'Ateneo G. D'Annunzio, Chieti per il triennio 2013-2015.

2016-2018 : Presidente del Nucleo di Valutazione dell'Ateneo G. D'Annunzio, Chieti per il triennio 2016-2018.

2019-2021 : Presidente del Nucleo di Valutazione dell'Ateneo G. D'Annunzio, Chieti per il triennio 2019-2021.

2018-2021 : Componente del Nucleo di Valutazione dell'Università Politecnica delle Marche, Ancona per il triennio 2018-2021.

2016-2019 : Presidente del Nucleo di Valutazione dell'Ateneo Telematico Leonardo da Vinci, Torrecchia Teatina (CH), per il triennio 2016-2019.

2013-2019 : Componente del direttivo del Coordinamento Nazionale Nuclei di Valutazione delle Università Italiane.

2015- : Inserito nell'Albo degli Esperti di Valutazione dell'ANVUR per il profilo di Esperti Disciplinari per la valutazione dei CdS.

2016 : Componente Commissione Esperti Valutatori (CEV) per i CdS di nuova istituzione per l'a.a. 2016/17. Inizio lavori della Commissione a marzo 2016 e termine a maggio 2016.

2016 : Componente Commissione Esperti Valutatori (CEV) per la visita ANVUR di Accreditamento degli Atenei e dei CdS – Università del Piemonte Orientale – Inizio lavori della Commissione a settembre 2016 e termine a maggio 2017.

2016-2018 : Componente della Commissione per l'Abilitazione Scientifica Nazionale nel Settore Concorsuale 03/B1 Chimica Generale ed Inorganica, nominata con DM del 31 ottobre 2016 ed in carica per due anni.

2017 : Componente Commissione Esperti Valutatori (CEV) per i CdS di nuova istituzione per l'a.a. 2017/18. Inizio lavori della Commissione a aprile 2017 e termine a maggio 2017.

2017 A far data dal 15 dicembre 2017 è stato iscritto dal Dipartimento della Funzione Pubblica all'albo nazionale dei componenti degli organismi indipendenti di valutazione (OIV) con attribuzione della **Fascia 2**- esperienza professionale di almeno otto anni negli ambiti indicati all'articolo 2, comma 1, lettera b), numero 2, del richiamato D.M., di cui tre come componente di Organismo indipendente di valutazione della performance o Nuclei di valutazione con funzioni analoghe.

2018 : Presidente di Commissione Esperti Valutatori (CEV) per i CdS di nuova istituzione per l'a.a. 2018/19. Inizio lavori della Commissione a aprile 2018 e termine a giugno 2018.

2018 : Componente Commissione Esperti Valutatori (CEV) per la visita ANVUR di Accreditamento degli Atenei e dei CdS – Università di Tor Vergata, ROMA – Inizio lavori della Commissione a marzo 2018 e termine a ottobre 2018.

2018 : Componente Commissione Esperti Valutatori (CEV) per la visita ANVUR di Accreditamento degli Atenei e dei CdS – Università Ca' Foscari, Venezia – Inizio dei lavori della Commissione a luglio 2018 e termine a dicembre 2018.

2019 : Componente Commissione Esperti Valutatori (CEV) per la visita ANVUR di Accreditamento degli Atenei e dei CdS – Università Milano Bicocca – Inizio dei lavori della Commissione a marzo 2019 e termine a settembre 2019.

2019 : Componente Commissione Esperti Valutatori (CEV) per la visita ANVUR di Accreditamento degli Atenei e dei CdS – Università dell’Insubria, Varese – Inizio dei lavori della Commissione a ottobre 2019.

2020 : Presidente Commissione Esperti Valutatori (CEV) per la visita ANVUR di Accreditamento degli Atenei e dei CdS – Università per gli Stranieri “Dante Alighieri”, Reggio Calabria – Inizio dei lavori della Commissione a marzo 2020 poi rinviato a ottobre 2020 causa emergenza COVID-19.

5. Qualificazione scientifica e culturale

Interessi scientifici:

Gli interessi scientifici del Prof. Nazzareno Re sono indirizzati verso la chimica inorganica teorica, ed in particolare i suoi temi di ricerca principali includono lo studio teorico dell'attivazione di piccole molecole su substrati inorganici o organometallici nella catalisi o in modelli di metalloenzimi, lo studio teorico della struttura elettronica e delle proprietà fisiche e chimiche di composti organometallici, lo studio teorico di processi su superfici di silice, fullereni e nanotubi, del comportamento magnetico di sistemi inorganici e metallorganici e lo studio teorico di complessi inorganici ed organometallici con proprietà antitumorali.

E' coautore di oltre duecento pubblicazioni scientifiche su riviste internazionali ed ha presentato i risultati delle sue ricerche in numerosi congressi internazionali.

I suoi indicatori bibliometrici (dati Scopus) dell'intera carriera sono:

n. pubblicazioni: 211

n. citazioni: 7009

h-index: 43

Gli indicatori bibliometrici (dati Scopus) di produzione scientifica previsti per la partecipazione alle commissioni per l'Abilitazione Scientifica Nazionale 2018 (art. 8 D.M. 120 del 7/6/2016 e D.M. 589 dell'8/8/2018) sono:

n. pubblicazioni ultimi 10 anni: 64

n. citazioni ultimi 15 anni: 2796

h-index ultimi 15 anni: 27

tutti e tre significativamente superiori alle soglie previste dal D.M. 589 dell'8/8/2018, rispettivamente: 53, 1663, 23.

E' revisore di numerose riviste scientifiche internazionali, tra le quali Journal of the American Chemical Society, Journal of Physical Chemistry A, B e C, Organometallics, Inorganic Chemistry, Dalton Transaction, Journal of Chemical Physics and Computation, Chemical Physics Letters

Dal 1999 è membro della American Chemical Society.

Attività Didattica:

Numerosa attività didattica di supporto nei Corsi di Laurea in Chimica e in Scienze Naturali presso la Facoltà di Scienze Matematiche Fisiche e Naturali dell'Università di Perugia dall'a.a. 1994/1995 all'a.a. 1997/1998.

Titolare del corso di Chimica Generale ed Inorganica del Corso di Laurea in C.T.F. della Facoltà di Farmacia dell'Università G. d'Annunzio dall'a.a. 1998/1999 all'a.a. 2015/16.

Titolare del corso di Chimica Generale ed Inorganica del Corso di Laurea in Farmacia della Facoltà di Farmacia dell'Università G. d'Annunzio negli a.a. 1998/1999, 1999/2000, 2000/2001 e 2009/2010.

Titolare del corso di Chimica Bioinorganica per i Corsi di Laurea in Farmacia e CTF della Facoltà di Farmacia dell'Università G. d'Annunzio dall'a.a. 2007/2008 all'a.a. 2015/16.

Supervisore di numerose Tesi di laurea e di Dottorato presso la Facoltà di Farmacia dell'Università G. d'Annunzio dall'a.a. 1998/99.

Membro e presidente di Commissione di numerosi Esami di Laurea nella Facoltà di Farmacia dell'Università G. d'Annunzio.

Componente del Collegio dei Docenti del Dottorato in Scienze del Farmaco dell'Università G. d'Annunzio dal XVI al XXVIII ciclo e del Collegio dei Docenti del Dottorato in Scienze Biomolecolari e Farmaceutiche dell'Università G. d'Annunzio dal XXIX al XXXII ciclo.

Membro di Commissione di diversi Esami finali di Dottorato nell'università G. d'Annunzio di Chieti-Pescara e nelle università di Roma Sapienza, Perugia, Pisa e Cosenza.

Attribuzione di incarichi di insegnamento o di ricerca (*fellowship*) ufficiale presso atenei e istituti di ricerca, esteri e internazionali, di alta qualificazione

- University of Lund (Sweden) gennaio-febbraio 1994 (Borsa di Ricerca breve CNR)
- Université de Lausanne (Suisse) aprile-luglio 1995 (Finanziamento Fond National Suisse)
- S.E.R.C.(Science and Engineering Research Center), Daresbury (UK) settembre - ottobre 1995 (Borsa di Ricerca Breve CNR)
- Université de Lausanne (Suisse) aprile-luglio 1996 (Borsa di Ricerca Fondation Herbette)
- Université de Lausanne (Suisse) novembre 1996 (Professore invitato)

- Université de Lausanne (Suisse) aprile-luglio 1997 (Borsa di Ricerca Fondation Herbette)
- Université de Paris Sud (France) aprile 1997 (Borsa di Ricerca Breve CNR)
- Université de Lausanne (Suisse) aprile-luglio 1998 (Borsa di Ricerca Fondation Herbette)
- Kumamoto University (Japan) agosto-ottobre 1998 (Finanziamento Ministero per la Ricerca del Giappone)
- Université de Lausanne (Suisse) dicembre 1998 (Professore invitato)
- Université de Lausanne (Suisse) giugno 2000 (Professore invitato)
- Kumamoto University (Japan) settembre-ottobre 2000 (Finanziamento Ministero per la Ricerca del Giappone)
- Dal 2001 ad oggi ha instaurato numerose collaborazioni scientifiche con diverse università italiane (Perugia, Firenze, Bari, Milano, Roma la Sapienza, Brescia, Palermo, Potenza, Ferrara) ed estere (Kumamoto, Giappone; Oita, Giappone; Okayama, Giappone; Paris Sud, Francia; Reims, Francia; Wroclaw, Polonia; Barcellona, Spagna; Madrid, Spagna; Aachen, Germania; Salvador, Brasile; Lund, Svezia) presso le quali ha effettuato numerose visite per motivi di ricerca ed ha tenuto diverse conferenze.

Data 23/05/2020

Nazzareno Re

ALLEGATO

Produzione Scientifica

Brevetti:

1. Deposito di domanda di brevetto in Italia, titolo:"Aerogel di Silice con legami Si-H", titolare: Istituto Guido Donegani Spa, Inventori designati: G. Cerofolini and **N. Re**, N. Domanda MI 91 A 002744, 1991 .

Publicazioni:

1. R. Colle, A. Fortunelli, **N. Re** and O. Salvetti, "Theoretical Investigation of the Ground and a Few Excited States of the Co(Schiff Base)Li Complexes", *J. Am. Chem. Soc.*, **1988**, *110*, 8016.
2. G.F. Cerofolini, A. Foglio Para and **N. Re**, "(D⁺D⁺)2e⁻ Binuclear Atoms as Activated Precursors in Cold and Warm Fusion" in S.E. Jones, F. Scaramuzzi and D. Worledge Eds. Anomalous Nuclear effects In Deuterium/Solids Systems, AIP Conference Proceedings 228, Provo UT 1990, pp. 668.
3. R. Colle, A. Fortunelli, **N. Re** and O. Salvetti, "Theoretical Investigation of the Ground and the Lowest Excited States of Co(SB) Complexes (SB=Schiff Base)", *Inorg. Chem.*, **1991**, *30*, 2388.
4. **N. Re**, "Kinetics of Bicomponent Sol-gel Processes", *J. Non-Cryst. Solids*, **1992**, *142*, 1.
5. **N. Re**, M. Rosi, A. Sgamellotti, C. Floriani and M.F. Guest, "Ab Initio Calculations on Methane Interacting with The Fourteen-electron Ni(PH₃)₂ Fragment", *J. Chem. Soc., Dalton Trans.*, **1992**, 1821.
6. V. Aquilanti, N. Nakamura, **N. Re** and C. Zhu, "The two-state linear curve crossing problem revisited. I. Analysis of Stokes phenomenon and expressions for scattering matrices", *J. Chem. Phys.*, **1992**, *97*, 1892.
7. **N. Re**, M. Rosi, A. Sgamellotti, C. Floriani and E. Solari, "A Theoretical Study of C-H Activation by LCu⁺ and LCu²⁺ Complexes", *J. Mol. Struct. (Theochem)* **1993**, 284, 95.
8. G.F. Cerofolini and **N. Re**, "The Mathematical Theory of Adsorption on Non-Ideal Surfaces", *La Rivista del Nuovo Cimento*, **1993**, *16*, 1.
9. E. Gallo, E. Solari, S. De Angelis, C. Floriani, **N. Re**, A. Chiesi-Villa and C. Rizzoli, "Four-centered oxotetramanganese(III)aggregate: a novel approach to redox and aggregation chemistry of manganese", *J. Am. Chem. Soc.*, **1993**, *115*, 9850.
10. G.F. Cerofolini and **N. Re**, "Bjerrum theory for hydrogen halides and noble-gas acids", *Gazz. Chim. Ital.*, **1993**, *123*, 653.
11. G.F. Cerofolini and **N. Re**, "Acid strength of XH_nH⁺ (n=0,4) ions", *Gazz. Chim. Ital.* **1993**, *123*, 653.
12. **N. Re**, M. Rosi, A. Sgamellotti and C. Floriani, "Theoretical Investigations and Modelling of Complex Inorganic Systems", in *Synthesis and Methodologies in Inorganic Chemistry*, S. Daolio, M. Fabrizio, P. Guerriero, E. Tondello, P.A. Vigato, Eds. (Bressanone, Italy, 1993), vol. 3, pp. 31.
13. **N. Re**, M. Rosi, A. Sgamellotti, C. Floriani and E. Solari, "A Theoretical Study of Dinitrogen Activation by V(II)and V(III): Ab initio Calculations on various model Compounds", *Inorg. Chem.*, **1994**, *33*, 4390.
14. **N. Re**, "Generalized local isotherm approximations", *J. Colloid Interf. Sci.*, **1994**, *166*, 191.
15. **N. Re**, A. Sgamellotti, B.J. Persson, B.O. Roos and C. Floriani, "A Theoretical Study of the (Cyclobutane)diazadivanadium Complex" *Organometallics*, **1995**, *14*, 63.
16. A. Klose, E. Solari, C. Floriani, A. Chiesi-Villa, C. Rizzoli and **N. Re**, " Magnetic Properties Diagnostic for the Existence of Iron(II)-Iron (II) Bonds in DinuclearComplexes Which Derive from Stepwise Insertion Reactions on Unsupported Iron-Aryl Bonds", *J. Am. Chem. Soc.*, **1994**, *116*, 9123.

17. G.F. Cerofolini and **N. Re**, "The Acid Bond", *Gazz. Chim. Ital.*, **1994**, *124*, 315.
18. **N. Re**, M. Rosi, A. Sgamellotti, and C. Floriani, "Theoretical Study of Dinitrogen Activation in Dinuclear V(II) and V(III) Hexacoordinated Complexes: Ab initio Calculations on Various Model Compounds", *Inorg. Chem.*, **1995**, *34*, 3410.
19. E. Solari, F. Musso, E. Gallo, C. Floriani, **N. Re**, A. Chiesi-Villa, and C. Rizzoli, "Cationic Aryl Manganese(II) Derivatives Occurring in Ion-Pair Forms with Tetraphenylborate Anions: Synthetic, Structural, and Magnetic Studies", *Organometallics*, **1995**, *14*, 2265.
20. G.F. Cerofolini and **N. Re**, "Extracting the Energy Distribution Function of Heterogeneous Surfaces from Their Desorption Kinetics", *J. Colloid Interf. Sci.*, **1995**, *174*, 428.
21. H. Miyasaka, N. Matsumoto, H. Okawa, **N. Re**, E. Gallo, and C. Floriani, "The Two-Dimensional Network Structure and Ferromagnetic Properties of the 2:1 Complex of [Mn(3-MeOsalen)(H₂O)]ClO₄ and K₃[Fe(CN)₆]", *Angew. Chem.*, **1995**, *34*, 1445.
22. H. Miyasaka, N. Matsumoto, H. Okawa, **N. Re**, E. Gallo, and C. Floriani, "Complexes Derived from the Reaction of Manganese(III) Schiff Base Complexes and Hexacyanoferrate(III): Syntheses, Multi-dimensional Network Structures, and Magnetic Properties", *J. Am. Chem. Soc.*, **1996**, *118*, 981.
23. P. Belanzoni, **N. Re**, M. Rosi, A. Sgamellotti, E.J. Baerends and C. Floriani, "Theoretical Investigations on Inorganic Systems and Aggregates by Density Functional Methods", In "Syntheses and Methodologies in Inorganic Chemistry - New Compounds and Materials", S. Daolio, E. Tondello, P.A. Vigato Eds., Bressanone (Italy), 1995, Vol. 5, p. 432.
24. P. Belanzoni, **N. Re**, M. Rosi, A. Sgamellotti, E.J. Baerends and C. Floriani, "Electronic Structure, Heisenberg Coupling Constants and Metal-Metal bond in Dimeric Iron(II) Organometallics with the Metal Centers at Variable Distances: a Density Functional Approach", *Inorg. Chem.*, **1996**, *35*, 7776.
25. P. Belanzoni, **N. Re**, M. Rosi, A. Sgamellotti, and C. Floriani, "Changes in the Interaction Mode of the Bridging "C₂" Units According to Transition Metal Parameters: a Theoretical Approach", *Organometallics*, **1996**, *15*, 4264.
26. G.F. Cerofolini and **N. Re**, "Kinetics of Desorption From Heterogeneous Surfaces", *Langmuir*, **1997**, *13*, 999.
27. E. Gallo, E. Solari, **N. Re**, C. Floriani, A. Chiesi-Villa, and C. Rizzoli, "Dioxygen Activation by a Manganese Complex Containing a Schiff-Base: Selective Oxidation of an Imino to an Amido Group Within the Salophen Ligand and Formation of a Hydroxy-Bridged Mn^{III}-Polymer", *Angew. Chem., Int. Ed. Engl.* **1996**, *35*, 1981.
28. E. Solari, A. Klose, C. Floriani, **N. Re**, A. Chiesi-Villa, and C. Rizzoli, "Design and X-ray Structure of a Planar Oxo Matrix for Binding Transition Metals: the Use of 2-Hydroxyisonaphthalic Acid as a Building Block for Planar Oxo Matrices", *Polyedron*, **1996**, *15*, 4103.
29. F. Franceschi, E. Gallo, E. Solari, C. Floriani, A. Chiesi-Villa, C. Rizzoli, **N. Re** and A. Sgamellotti, "Synthetic Methodology Allowing the Interconversion of Titanium-Oxygen Single Bonds and Double Bonds: the Self-Assembling of Bridging and Terminal Oxotitanium(IV) into Oligomeric and Polymeric Linear Titanoxanes", *Chem. Eur. J.*, **1996**, *2*, 1466.
30. **N. Re**, A. Sgamellotti, and C. Floriani, "Theoretical Study of [Fe(CO)₂Cp]₃(μ₃-C₃)⁺ Tricarbido Cation", *Organometallics*, **1996**, *15*, 5330.
31. **N. Re**, E. Gallo, and C. Floriani, H. Miyasaka, N. Matsumoto, "Anomalous Magnetic Properties of K[Mn(3-MeOsalen)][Mn(CN)₆]: a Metamagnet Exhibiting a Strong Negative Magnetization 3-MeOsalen=N,N'-ethylenbis(3-methoxysalicylideneiminato)", *Inorg. Chem.*, **1996**, *35*, 5694.
32. **N. Re**, E. Gallo, C. Floriani, H. Miyasaka and N. Matsumoto, "Magnetic Properties of One-Dimensional Ferromagnet containing a Mn(III)-CN-Fe(III) Linkage, Synthesis and Crystal Structure of a Chainlike [Mn(acacen)][Fe(CN)₆]_n²ⁿ⁻ Polyanion", *Inorg. Chem.*, **1996**, *35*, 6004.

33. H. Miyasaka, N. Matsumoto **N. Re**, E. Gallo, and C. Floriani, "Synthesis, Crystal Structure and Magnetic Properties of a Ferrimagnet Layered Compound $[\text{NEt}_4]_2[\text{Mn}(5\text{-Cl-salen})][\text{Fe}(\text{CN})_6]$, 5-Cl salen=N,N'-ethylenebis((5-chlorosalicylidene)aminato)", *Inorg. Chem.*, **1997**, *36*, 670.
34. P. Belanzoni, S. Fantacci, **N. Re**, M. Rosi, A. Sgamellotti, and C. Floriani, "Oligomerization of the $\text{PH}_3\text{Cu-C}\equiv\text{C-CuPH}_3$ Acetylide toward the Formation of PH_3CuC ($n=4,6,8$) Metal Carbides: a Theoretical Study Based on Density Functional Theory", *Inorg. Chem.*, **1997**, *36*, 2018.
35. E. Gallo, E. Solari, **N. Re**, C. Floriani, A. Chiesi-Villa and C. Rizzoli, "Carbon-Carbon Bonds Functioning as Electrons Shuttles: the Generation of Electron-Rich Manganese(II)-Schiff Base Complexes and their Redox Chemistry", *J. Am. Chem. Soc.*, **1997**, *119*, 5144.
36. L. Giannini, A. Caselli, E. Solari, C. Floriani, A. Chiesi-Villa, C. Rizzoli, **N. Re** and A. Sgamellotti, "Organometallic Reactivity on a Calix[4]arene Oxo Surface. Synthesis and Rearrangement of Zr-C Functionalities Anchored to a Calix[4]arene Moiety", *J. Am. Chem. Soc.*, **1997**, *119*, 9198.
37. L. Giannini, A. Caselli, E. Solari, C. Floriani, A. Chiesi-Villa, C. Rizzoli, **N. Re** and A. Sgamellotti, "Organometallic Reactivity on a Calix[4]arene Oxo Surface. The Stepwise Migratory Insertion of Carbon Monoxide and Isocyanides into Zirconium-Carbon Bonds Anchored to a Calix[4]arene Moiety", *J. Am. Chem. Soc.*, **1997**, *119*, 9709.
38. F. De Angelis, **N. Re**, M. Rosi, A. Sgamellotti, and C. Floriani, "A theoretical study of acetylide complexes of early transition metals", *J. Chem. Soc., Dalton*, **1997**, 3841.
39. N. Re, A. Sgamellotti, G.F. Cerofolini and L. Meda, "Theoretical Analysis of CO_2 Adducts to the Native E' Centre in Ion-bombarded Porous Silica", *J. Phys. Chem.*, **1997**, *101*, 9695.
40. S. Fantacci, **N. Re**, M. Rosi, A. Sgamellotti, M. Guest, P. Sherwood, and C. Floriani, "A theoretical study of the metathesis-like reaction between ditungsten hexaalkoxydes and alkynes", *J. Chem. Soc., Dalton Trans.*, **1997**, 3845.
41. A. Klose, E. Solari, C. Floriani, **N. Re**, A. Chiesi-Villa, and C. Rizzoli, "Iron-carbene functionalities supported by a macrocyclic ligand: iron-carbon double bond stabilized by tetramethyldibenzotetraazaannulene", *J. Chem. Soc., Chem. Comm.*, **1997**, 2297.
42. R. Ferguson, E. Solari, C. Floriani, D. Osella, M. Ravera, **N. Re**, A. Chiesi-Villa, and C. Rizzoli, "The Stepwise Reduction of Dinitrogen Occurring on a Divanadium Model Compound: A Synthetic, Structural, Magnetic and Theoretical Investigation on the $[\text{V}=\text{N}=\text{N}=\text{V}]^{n+}$ [$n=4-6$] Based Complexes", *J. Am. Chem. Soc.*, **1997**, *119*, 10104.
43. P. Belanzoni, **N. Re**, A. Sgamellotti, and C. Floriani, "Interaction mode of the bridging c_2 unit in dinuclear complexes of late transition metals in low oxidation states: a theoretical approach", *J. Chem. Soc., Dalton Trans.*, **1997**, 4773.
44. A. Caselli, L. Giannini, E. Solari, C. Floriani, **N. Re**, A. Chiesi-Villa, and C. Rizzoli, "Zirconium-Butadiene Bonded over a Planar Set of Oxygens Derived from Calix[4]arene and its Behavior as a Source of Zirconium(II)", *Organometallics*, **1997**, *16*, 5457.
45. A. Zanotti-Gerosa, L. Giannini, E. Solari, C. Floriani, **N. Re**, A. Chiesi-Villa, and C. Rizzoli, "Titanium-Carbon Functionalities on an Oxo Surface Defined by a Calix[4]arene Moiety and its Redox Chemistry", *Inorg. Chim. Acta* **1998**, *270*, 298.
46. P. Belanzoni, **N. Re**, A. Sgamellotti, and C. Floriani, "Electronic communication between carbon chain bridged metals: a theoretical approach. Even chains", *J. Chem. Soc., Dalton Trans.* **1998**, 1825.
47. **N. Re**, A. Sgamellotti, and C. Floriani, " $[(\text{L})_n\text{M-C}_m^-]_x$: Hypothetical organometallic polymers with metallapolyine and metallacumulene character", *J. Chem. Soc., Dalton Trans.*, **1998**, 2521.
48. H. H. Miyasaka, H. Ieda, and N. Matsumoto **N. Re**, R. Crescenzi, and C. Floriani, "Assembling Bi-, Tri-, and Pentanuclear Complexes into Extended Structures Using a Desolvation Reaction: Synthesis,

Structure and Magnetic Properties of Manganese(III)-Schiff-Base-Hexacyanoferrate Polymeric Compounds and Their Derived Extended Structures", *Inorg. Chem.* **1998**, *37*, 255.

49. **N. Re**, R. Crescenzi, C. Floriani, H. Miyasaka, and N. Matsumoto "The Synthesis and Characterization of Two Dimensional Ferromagnetic Extended Structures Containing High Spin ($S=5/2$) and Low Spin ($S=1/2$) Iron(III) Bridged by Cyanide Groups", *Inorg. Chem.* **1998**, *37*, 2717.
50. F. De Angelis, **N. Re**, A. Sgamellotti, A. Selloni, J. Weber, and C. Floriani, "A dynamical density functional study of CO migration in the Reppe carbonylation", *Chem. Phys. Lett.* **1998**, *291*, 57.
51. U. Piarulli, C. Floriani, **N. Re**, G. Gervasio and D. Viterbo, "Diacetoneglucose Complexes of Manganese(II) and Iron(II) and Their Organometallic Derivatization", *Inorg. Chem.*, **1998**, *37*, 5142.
52. H. Y. Sunatsuki, H. Shimada, M. Nakamura, F. Kai, N. Matsumoto, and **N. Re**, "Synthesis, Magnetic Property and Incomplete Double-Cubane Structure of Manganese(III)-Metal(II) Complexes $[Mn(MeOH)L(OH)M(bpy)]_2$: ($M=Zn,Cu,Ni$ and Mn ; $H_4L=1,2$ Bis(2-hydroxybenzamido)benzene; $bpy=2,2'$ -Bipyridine", *Inorg. Chem.*, **1998**, *37*, 5566.
53. B. Castellano, E. Solari, C. Floriani, **N. Re**, A. Chiesi-Villa, and C. Rizzoli, "The Chemistry of Vanadium-Carbon Bond Functionalities over an Oxo-Surface Defined by the Calix[4]arene Skeleton: The Redox Relationship between Vanadium(III) and Vanadium(IV) Assisted by Carbon-Oxygen Bond Cleavage", *Organometallics*, **1998**, *17*, 2328.
54. H. M. Mimura, T. Matsuo, N. Matsumoto, S. Takamizawa, W. Mori and **N. Re**, "Di- μ -phenoxobis[(N-salicylidene-N'-(2-phenylimidazol-4-ylmethylidene)1,3-propanediamino)(methanol)nickel(II)] Perchlorate and the Deprotonated Imidazolate-Bridged Cyclic-Tetranuclear Complexes: Synthesis, Property and Structure", *Bull. Chem. Soc. Jpn.*, **1998**, *71*, 1831.
55. G.F. Cerofolini, **N. Re**, "Chemical perspectives on growth and properties of ultrathin SiO_2 layers" E. Garfunkel et al. Eds., "Fundamental aspects of ultrathin dielectric on Si-based Devices", Kluwer Academic Publisher; Amsterdam: 1998, pp. 117.
56. **N. Re**, A. Sgamellotti and G.F. Cerofolini, "Theoretical Analysis of ethylene adducts to the Native E' centre in Ion-bombarded Porous Silica", *Int. J. Mass Spectr.*, **1999**, *180*, 27.
57. H. N. Matsumoto, Y. Motoda, T. Matsuo, T. Nakashima, **N. Re**, F. Dahan, J.-P. Tuchagues, "Proton-Dependent Monomer-Oligomer Interconversion of Copper(II) Complexes with N-(2-R-imidazol-4-ylmethylidene)-2-aminoethylpyridine ($R=$ Methyl and Phenyl)" *Inorg. Chem.* **1999**, *38*, 1165.
58. F. Nunzi, A. Sgamellotti, **N. Re** and C. Floriani, "A density functional study of $[M(PH_3)_2(\eta^2-C_2X_4)]$ alkene complexes for the Group 10 metals: the effect of electron-attracting substituents", *J. Chem. Soc., Dalton Trans.* **1999**, 3487.
59. A. Klose, E. Solari, J. Hesschenbrouck, C. Floriani, **N. Re**, S. Geremia and L. Randaccio, "Ruthenium-Carbene Functionality Bonded to Dibenzotetramethyltetraaza[14]annulene: Metal-to-Macrocyclic Ligand-Induced Carbene Migration", *Organometallics* **1999**, *18*, 360.
60. B. Castellano, E. Solari, C. Floriani, **N. Re**, A. Chiesi-Villa and C. Rizzoli, "Tantalum-Carbon Functionalities Bonded to a Calix[4]arene-Oxo Matrix: the Chemistry of Mono-, Dialkyl and Butadiene Derivatives of Tantalum(V)", *Chem. Eur. J.* **1999**, *5*, 722.
61. R. Crescenzi, E. Solari, C. Floriani, **N. Re**, A. Chiesi-Villa and C. Rizzoli, "Metal-Porphyrinogen Organometallic Chemistry: the Intramolecular Reactivity of η^2 -Acyls Bonded to Titanium(IV)-*meso*-Octaethyl Mono(pyridine)-Tris(pyrrole) and to Vanadium(III)-*meso*-Octaethyl Bis(pyridine)-Bis(pyrrole) Macrocyclic", *Organometallics* **1999**, *18*, 606.
62. L. Giannini, E. Solari, C. Floriani, **N. Re**, A. Chiesi-Villa and C. Rizzoli, "Tungsten-Tungsten Multiple Bond Functionalities Supported by a Polyoxo Surface Modeled by Calix[4]arene", *Inorg. Chem.* **1999**, *38*, 1438.

63. L. Giannini, E. Solari, S. Dovesi, C. Floriani, **N. Re**, A. Chiesi-Villa and C. Rizzoli, "Genesis, Redox and Acid-Base Relationships among W-C, W=C, W≡C Functionalities over an Oxo Surface Modeled by Calix[4]arene", *J. Am. Chem. Soc.* **1999**, *121*, 2784.
64. L. Giannini, G. Guillemot, E. Solari, C. Floriani, **N. Re**, A. Chiesi-Villa and C. Rizzoli, "Olefin Rearrangements Assisted by a Molecular Metal-Oxo Surface: The Chemistry of Calix[4]arene-Tungsten(IV)", *J. Am. Chem. Soc.* **1999**, *121*, 2797.
65. B. Castellano, E. Solari, C. Floriani, R. Scopelliti and **N. Re**, "Reactivity of a Vanadium(III) Center over an Oxo Surface Modeled by Calix[4]arene", *Inorg. Chem.* **1999**, *38*, 3406.
66. A. Klose, J. Hesschenbrouck, E. Solari, C. Floriani, **N. Re**, A. Chiesi-Villa and C. Rizzoli, "The Metal-Carbon Multiple Bond in Iron(I)- and Iron(II)-Dibenzotetramethyltetra[14]azaannulene: Carbene, Carbonyl, and Isocyanide Derivatives", *J. Organometal. Chem.* **1999**, *591/1-2*, 45.
67. F. Mercuri, **N. Re**, and A. Sgamellotti, "Influence of substituents and lengths of silanylene units on the electronic structure of π -conjugated polymeric organosilicon systems", *Theochem-J. Mol. Struct.* **1999**, *489*, 35.
68. H. Y. Sunatsuki, H. Shimada, M. Nakamura, F. Kai, N. Matsumoto, and **N. Re**, "Synthesis, Magnetic Property and Incomplete Double-Cubane Structure of Manganese(III)-Metal(II) Complexes [Mn(MeOH)L(OH)M(bpy)]₂: (M=Zn,Cu,Ni and Mn; H₄L=1,2Bis(2-hydroxybenzamido)benzene; bpy=2.2'-Bipyridine)", *Inorg. Chem.*, **1999**, *38*, 2756.
69. J. Hesschenbrouck, E. Solari, C. Floriani, **N. Re**, C. Rizzoli and A. Chiesi-Villa "Chromium-(II) and -(III) over a planar oxo surface modelled by calix[4]arene anions: redox chemistry and formation of Cr-C functionalities", *J. Chem. Soc., Dalton Trans.* **2000**, 191.
70. C. Stern, F. Franceschi, E. Solari, C. Floriani, **N. Re** and R. Scopelliti, "The use of macrocyclic and polydentate ligands in ruthenium organometallic chemistry", *J. Organomet. Chem.*, **2000**, *593-594*, 86.
71. J. Hesschenbrouck, E. Solari, R. Scopelliti, C. Floriani, and **N. Re**, "The metal-metal bond in the dibenzotetramethyltetraaza[14]annulene-ruthenium dimer: a structural, magnetic, and theoretical analysis", *J. Organomet. Chem.* **2000**, *596/1-2*, 77.
72. F. Franceschi, J. Hesschenbrouck, E. Solari, C. Floriani, **N. Re**, C. Rizzoli and A. Chiesi-Villa, "The reactivity of dibenzotetramethyltetraaza[14]annulene-Mn(II): functionalisation of manganese in a macrocyclic environment", *J. Chem. Soc., Dalton Trans.*, **2000**, 593.
73. P. Belanzoni, A. Sgamellotti, **N. Re**, and C. Floriani, "Oligomerization of Early Transition Metal {M(OH)₃}₂(μ -C₂) Acetylides toward the Formation of [(OH)₃MC]_n (n = 4,6) Metalla Carbides: A Theoretical Study by Density Functional Theory", *Inorg. Chem.* **2000**, *39*, 1147.
74. **N. Re**, A. Sgamellotti, and C. Floriani, "Density Functional Study of metallacumulene Complexes", *Organometallics* **2000**, *19*, 1115.
75. A. Caselli, E. Solari, R. Scopelliti, C. Floriani, **N. Re**, C. Rizzoli and A. Chiesi-Villa, "Dinitrogen Rearranging over a Metal-Oxo Surface and Cleaving to Nitride: From the End-On to the Side-On Bonding Mode, to the Stepwise Cleavage of the N≡N Bonds Assisted by Nb^{III}-calix[4]arene", *J. Am. Chem. Soc.* **2000**, *122*, 3652.
76. F. Nunzi, A. Sgamellotti, **N. Re**, and C. Floriani, "A Density Functional Study of C₆₀ Transition Metal Complexes", *Organometallics* **2000**, *19*, 1628.
77. L. Bonomo, E. Solari, R. Scopelliti, C. Floriani, and **N. Re**, "The Porphyrinogen-Porphodimethene Relationship Leading to Novel Synthetic Methodologies Focused on the Modification and Functionalization of the Porphyrinogen and Porphodimethene Skeletons", *J. Am. Chem. Soc.* **2000**, *122*, 5312.
78. V. Esposito, E. Solari, C. Floriani, **N. Re**, C. Rizzoli and A. Chiesi-Villa, "Binding and Redox Properties of Iron(II) Bonded to an Oxo-Surface Modeled by Calix[4]arene", *Inorg. Chem.* **2000**, *39*, 2604.

79. G.F. Cerofolini, A. P. Caricato, L. Meda, **N. Re** and A. Sgamellotti, "Quantum mechanical study of nitrogen bonding configurations at the nitrated Si-SiO₂ interface *via* model molecules", *Phys. Rev. B* **2000**, *61*, 14157.
80. G.F. Cerofolini, L. Meda, **N. Re**, "Adsorption on Ion-Bombarded Silica", E. Papirer Ed., Adsorption on Silica Surfaces, Marcel Dekker; New York: **2000**; p. 369
81. G.F. Cerofolini, L. Meda, **N. Re**, "Core electrons as probes of the net atomic charge. A theoretical and experimental investigations", *Res. Adv. In Physical Chem.* **2000**, *1*, 77.
82. F. De Angelis, A. Sgamellotti, and **N. Re**, "Density functional study of the Reppe carbonylation of acetylene", *Organometallics* **2000**, *19*, 4104.
83. F. De Angelis, A. Sgamellotti, and **N. Re**, "Density functional study of the CO Insertion into the Metal-Alkyl bond in bis(cyclopentadienyl)-Zr-(CH₃)(2)", *Organometallics* **2000**, *19*, 4904.
84. G. Guillemot, E. Solari, C. Floriani, **N. Re** and C. Rizzoli, "Alkene and Alkyne Reactivity over a metal-oxo surface modeled by Calix[4]arene-Tungsten(IV): Formation of 1-metallacyclopropene and alkylidene complexes", *Organometallics*, **2000**, *19*, 5218.
85. C. Da Silva, L. Bonomo, E. Solari, R. Scopelliti, C. Floriani, and **N. Re**, "The Binding Ability of Iron Bonded to Porphodimethene: Structural, Magnetic and Electronic Relationship with Iron-Porphyrin", *Chem. Eur J.* **2000**, *6*, 4318.
86. E. Solari, J. Hesschenbrouck, R. Scopelliti, C. Floriani, and **N. Re**, "From Oligomers to Conducting Polymers of the Metal dinitrogen Functionality ", *Angew. Chem. Int. Ed. Engl.* **2001**, *40*, 932.
87. G.F. Cerofolini and **N. Re** "Core electrons as probes of the Net-Charge Distribution in Molecules. A Case Study", *Chem. Phys. Lett.* **2001**, *333*, 181.
88. S. Fantacci, A. Sgamellotti, C. Floriani and **N. Re**, "A Density functional study of tetraphenolate and calix[4]arene complexes of early transition metals", *Inorg. Chem.* **2001**, *40*, 1544.
89. G.F. Cerofolini and **N. Re** "Studies in Acis-Base Theory. The base Strength of Amines.", *Chem. Phys. Lett.* **2001**, *339*, 375.
90. F. De Angelis, A. Sgamellotti, and **N. Re**, "Density functional study of the CO Insertion into the Metal-Alkyl bond in bis(cyclopentadienyl)-Ti-(CH₃)(2)", *J. Chem. Soc, Dalton Trans.* **2001**, 1023.
91. F. De Angelis, A. Sgamellotti, and **N. Re**, "Density functional study of the CO Insertion into the Metal-Alkyl bond in bis(cyclopentadienyl)-Zr-(CH₃)(2)", *Organometallics* **2001**, *20*, 1406.
92. G.F. Cerofolini, L. Meda and **N. Re** "A method for the experimental determination of the net atomic charge via X-ray photoemission spectroscopy ", *Appl. Phys. A* **2001**, *72*, 603.
93. F. Franceschi, G. Guillemot, E. Solari, C. Floriani, H. Birkedal **N. Re** and P. Pattison , "Reduction of Dioxygen by a Dimanganese Unit Bonded inside a Cavity Provided by a Pyrrole-Based Dinucleating Ligand ", *Chem. Eur. J.*, **2001**, *7*, 1468.
94. S. Fantacci, A. Sgamellotti, C. Floriani and **N. Re**, "A density functional study of Ethylene rearrangements assisted by tungsten calix[4]arene", *J. Chem. Soc, Dalton Trans.* **2001**, 1718.
95. F. De Angelis, S. Fantacci, A. Sgamellotti, C. Floriani and **N. Re**, "Dynamical density functional study of the multistep CO Insertion into the Metal-Carbon bond in (Calix[4]arene)-Zr-Me₂", *Organometallics.* **2001**, *20*, 4031.
96. N. Re, L. Bonomo, C. Da Silva, E. Solari, R. Scopelliti, and C. Floriani, "A Structural and Theoretical Analysis of Transition Metal Porphodimethene and Their Relationship with Metalloporphyrins", *Chem., Eur. J.* , **2001**, *7*, 2536.
97. F. Nunzi, A. Sgamellotti, **N. Re**, "A Density Functional Study of Carbon-Carbon Bond Activation in Curved Aromatic Hydrocarbons by Transition Metal Complexes", *Organometallics.* **2002**, *21*, 2219.

98. F. De Angelis, A. Sgamellotti and **N. Re**, "Four and five coordinate CO insertion in the copolymerization of carbon monoxide and olefins catalyzed by diphosphine nickel(II) complexes: a dynamical density functional study", *Organometallics*, **2002**, *21*, 2036.
99. N. Re and G. F. Cerofolini, "Heterolytic dissociation under hot-electrons bombardment of the silanic bond at the Si-SiO₂ interface", *Appl. Phys. A*, **2002**, *74*, 599-603.
100. F. De Angelis, A. Sgamellotti and N. Re, "A dynamical density functional study of acetylene to vinylidene isomerization in (Cp)(CO)₂Mn(HC≡CH)", *Organometallics*, **2002**, *21*, 2715.
101. F. Nunzi, A. Sgamellotti, **N. Re**, "A Pyracylene Model for the Interaction of Transition Metal Complexes: A Density Functional Study", *J. Chem. Soc., Dalton Trans.* **2002**, 399.
102. P. Belanzoni, **N. Re**, A. Sgamellotti, and C. Floriani, "Electronic communication between carbon chain bridged metals: a theoretical approach. Odd chains", *J. Organomet. Chem.* **2002**, *656*, 156-167.
103. F. Mercuri, A. Sgamellotti, **N. Re**, "A density functional theory study of bridging and terminal oxotitanium(IV) oligomeric and polymeric linear titanoxanes", *Theor. Chem. Acc.* **2002**, *108*, 46-52
104. Francesca Nunzi, Antonio Sgamellotti, **Nazzareno Re**, "The Coordination Chemistry of Carbon Nanotubes: a Density Functional Study through a Cluster Model Approach", *J. Phys. Chem. B* **2002** *106*, 10622-10633.
105. Alessandro Marrone, **N. Re**, "Effects of Terminal Substituents on Metallacumulene Complexes: A Density Functional Study on (CO)₅Cr(=C)_nX₂ (X = F, SiH₃, CHCH₂, NH₂, NO₂)", *Organometallics* **2002**, *21*, 3562-3571.
106. Cerofolini, G. F.; Marrone, A.; Re, Nazzareno "Correlating proton affinity and HOMO energy of neutral and negatively charged bases" *Theochem* **2002**, *588*, 227-232.
107. Giorgi, Giacomo; De Angelis, Filippo; Re, Nazzareno; Sgamellotti, Antonio "Oxidative addition of SiH₄ to Pt(PH₃)₂: a dynamical density functional study" *Chemical Physics Letters* **2002**, *364*, 87-92.
108. Simona; De Angelis, Filippo; Sgamellotti, Antonio; Re, Nazzareno. "A Dynamic Density Functional Study of the Stepwise Migratory Insertion of Isocyanides into Zirconium-Carbon Bonds Anchored to a Calix[4]arene Moiety" *Organometallics* **2002**, *21*, 4090-4098.
109. De Angelis, Filippo; Sgamellotti, Antonio; Re, Nazzareno "Density Functional Study of Alkyne to Vinylidene Rearrangements in [(Cp)(PMe₃)₂Ru(HC≡CR)]⁺ (R= H, Me)" *Organometallics* **2002**, *21*, 5944-5950.
110. Giorgi, Giacomo; De Angelis, Filippo; **Re, Nazzareno**; Sgamellotti, Antonio "A density functional study on the Pt(0)-catalysed hydrosilylation of ethylene" *Theochem* **2003**, *623*, 277-288.
111. Kido, Takafumi; Ikuta, Yuichi; Sunatsuki, Yukinari; Ogawa, Yoshihiro; Matsumoto, Naohide; **Re, Nazzareno** "Nature of Copper(II)-Lanthanide(III) Magnetic Interactions and Generation of a Large Magnetic Moment with Magnetic Anisotropy of 3d-4f Cyclic Cylindrical Tetranuclear Complexes [CuII LnIII(hfac)₂]₂, (H₃L = 1-(2-Hydroxybenzamido)-2-(2-hydroxy-3-methoxybenzylideneamino)ethane and Hhfac = Hexafluoroacetylacetone, LnIII = Eu, Gd, Tb, Dy)" *Inorg. Chem.* **2003**, *42*, 398-408.
112. Nakamura, Masaaki; Kawachi, Minako; Konatsu, Chikako; Osa, Shutaro; Tarui, Takao; Matsumoto, Naohide; **Re, Nazzareno** "Syntheses and magnetic properties of cyclic tetranuclear and infinite linear-chain copper(II)-manganese(II) complexes" *Chemistry Letters* **2003**, *32*, 936-937.
113. De Angelis, Filippo; Fantacci, Simona; Sgamellotti, Antonio; **Re, Nazzareno** "The migratory insertion of carbon monoxide and methyl isocyanide into zirconium-carbon and titanium-carbon bonds anchored to a calix[4]arene moiety: a dynamical density functional study" *T. C. A.* **2003**, *110*, 196-204.
114. Osa, Shutaro; Sunatsuki, Yukinari; Yamamoto, Yoko; Nakamura, Masaaki; Shimamoto, Tomoshige; Matsumoto, Naohide; **Re, Nazzareno** "Synthesis and Magnetic Properties of Heterometal Cyclic Tetranuclear Complexes [CuII MII(hfac)₂] (MII = Zn, Cu, Ni, Co, Fe, Mn; H₃L = 1-(2-

Hydroxybenzamido)-2-((2-hydroxy-3-methoxybenzylidene)amino)ethane; Hhfac = Hexafluoroacetylacetone)." *Inorg. Chem.* **2003**, *42*, 5507-5512.

115. Cerofolini, G. F.; Galati, C.; Renna, L.; **Re, N.** "The early oxynitridation stages of hydrogen-terminated (100) silicon after exposure to N₂:N₂O. II. Silicon and oxygen bonding states" *Appl. Phys. A: Materials Science & Processing*, **2003**, *77*, 515-521.
116. Giorgi, Giacomo; De Angelis, Filippo; **Re, Nazzareno**; Sgamellotti, Antonio "A density functional study on the Pt(0)-catalyzed hydrosilylation of ethylene" *Theochem* **2003**, *623*, 277-288.
117. Francesca Nunzi, Francesco Mercuri, Filippo De Angelis, Antonio Sgamellotti, **Nazzareno Re**, Paolo Giannozzi "Coordination and Haptotropic Rearrangement of Cr(CO)₃ on (n,0) Nanotube Sidewalls: A Dynamical Density Functional Study", *J. Phys. Chem. B* **2004** *108*, 5243-5249.
118. Osa, Shutaro; Kido, Takafumi; Matsumoto, Naohide; **Re, Nazzareno**; Pochaba, Andrzej; Mrozinski, Jerzy "A Tetranuclear 3d-4f Single Molecule Magnet: [Cu^{II}LTb^{III}(hfac)₂]₂." *J. Am. Chem. Soc.* **2004**, *126*, 420-421.
119. Francesca Nunzi, Antonio Sgamellotti, **Nazzareno Re**, "Density Functional Study on the Interaction of a Polycyclic Aromatic Molecule and the Silicon (001) Surface", *J. Phys. Chem. B* **2004** *108*, 10881-10886.
120. Cerofolini, G. F.; Foglio, P.; **Re, N.** "Binuclear atoms. I. A semiphenomenological treatment" *Recent Res. Devel. Physics*, **2004**, *5*, 347-368.
121. De Angelis, Filippo; Sgamellotti, Antonio; Re, Nazzareno "Density Functional Study of Alkyne to Vinylidene Rearrangements in d⁶ complexes" *J. Chem. Soc.; Dalton Transaction*, **2004**, 3225-3230.
122. Alessandro Marrone, Cecilia Coletti, **N. Re**, "Metal Fragment Modulation of Metallacumulene Complexes: A Density Functional Study", *Organometallics* **2004**, *23*, 4952-4963.
123. Yagamuchi, T.; Sunatsuki, Y; Kojima, M.; Akashi, H.; Tsuchimoto, M.; Re, N.; Shutaro, O.; Matsumoto, N. "Ferromagnetic NiII-GdIII interactions in complexes with NiGd, NiGdNi, and NiGdGdNi cores supported by tripodal ligands" *J. Chem. Soc.; Chem. Comm.*, **2004**, 1048-1049.
124. De Angelis, Filippo; Fantacci, Simona; Sgamellotti, Antonio; Re, Nazzareno "A TDDFT study of the ruthenium(II) polycyclic aromatic complex [Ru(dppz)(phen)₂]²⁺ in solution" *Chem. Phys. Lett.* **2004**, *396*, 43-48.
125. De Angelis, Filippo; Sgamellotti, Antonio; Re, Nazzareno; Fantacci, Simona "Intramolecular Coupling of η²-Iminoacyls on Zirconium Bis(aryloxides) and Calix[4]arenes: Revised Mechanism by DFT Calculations and Car-Parrinello Molecular Dynamics Simulations" *Organometallics* **2005**, *24*, 1867-1875.
126. Fantacci, S.; De Angelis, F.; Sgamellotti, A.; Marrone, A.; **Re, N.** "Photophysical properties of [Ru(phen)₂(dppz)]²⁺ intercalated into DNA: an integrated Car-Parrinello and TDDFT study" *J. Amer. Chem. Soc.*, **2005**, *127*, 14144-14145.
127. Nunzi, Francesca; Sgamellotti, Antonio; **Re, Nazzareno** "Selective functionalization of the Si(100) surface by a bifunctional alkynilamine molecule: A density functional study of the switching adsorption linkage" *Chem. Phys. Lett.* **2005**, *413*, 473-478.
128. Yamada, Masahiro; Fukumoto, Eri; Ooidemizu, Makoto; Brefuel, Nicolas; Matsumoto, Naohide; Iijima, Seiichiro; Kojima, Masaaki; **Re, Nazzareno**; Dahan, Françoise; Tuchagues, Jean-Pierre "A 2D Layered Spin Crossover Complex Constructed by NH...Cl- Hydrogen Bonds: [FeIIH₃LMe]Cl·I₃ (H₃LMe = Tris[2-(((2-methylimidazolyl-4-yl)methylidene)amino) ethyl]amine" *Inorg. Chem.* **2005**, *44*, 6967-6974.
129. Cerofolini, G. F.; Galati, C.; Reina, S.; Renna, L.; Condorelli, G. G.; Fragala, I. L.; Giorgi, G.; Sgamellotti, A.; **Re, N.** "Functionalization of atomically flat, dihydrogen terminated, 1x1 (100) silicon via reaction with 1-alkyne" *Appl. Surf. Sci.* **2005**, *246*, 52-67.

130. Nunzi, F.; Sgamellotti, A.; **Re, N.** "Selective Functionalization of the Si(100) Surface by a Bifunctional Alkynylamine Molecule: Density Functional Study of the Switching Adsorption Linkage. 2" *J. Phys. Chem. B*. **2006**, *110*, 7682-7687.
131. D. Bellocchi, G. Costantino, R. Pellicciari, **N. Re**, A. Marrone, C. Coletti "Poly(ADP-Ribose)-Polymerase-Catalyzed Hydrolysis of NAD⁺: QM/MM simulation of the Enzyme Reaction", *ChemMedChem*, **1** (2006), 533-539.
132. C. Coletti and **N. Re** "Theoretical Study of Alkali-Benzene Complexes: Potential Energy Surfaces and Binding Energies with Improved Results for Rubidium and Cesium", *J. Phys. Chem. A*, **110** (2006), 6563-6570.
133. M. Albertí, A. Aguilar, J. M. Lucas, F. Pirani, D. Cappelletti, C. Coletti and **N. Re**, "Atom-bond Pairwise Additive Representation for Cation-Benzene Potential Energy Surfaces: an Ab Initio Validation Study", *J. Phys. Chem. A*, **110** (2006), 9002-9010.
134. C. Coletti, A. Marrone, G. Giorgi, A. Sgamellotti, G. Cerofolini, and N. Re "Non-radical mechanisms for the uncatalyzed thermal functionalization of silicon surfaces by alkenes and alkynes: A density functional study", *Langmuir*, **22** (2006), 9949-9956.
135. Yamada, Masahiro; Hagiwara, Hiroaki; Torigoe, Haruna; Matsumoto, Naohide; Kojima, Masaaki; Dahan, Françoise; Tuchagues, Jean-Pierre; Re, Nazzareno; Iijima, Seiichiro. "A variety of spin-crossover behaviors depending on the counter anion: two-dimensional complexes constructed by NH⁺...Cl⁻ hydrogen bonds, [Fe^{II}H₃LMe]ClX (X = PF₆⁻, AsF₆⁻, SbF₆⁻, CF₃SO₃⁻; H₃LMe = tris[2-[[[2-methylimidazol-4-yl)methylidene]amino]ethyl] amine)." *Chemistry--A European Journal*, **12** (2006), 4536-4549.
136. Kobayashi, Tamami; Yamaguchi, Tomoka; Ohta, Hiromi; Sunatsuki, Yukinari; Kojima, Masaaki; **Re, Nazzareno**; Nonoyama, Matsuo; Matsumoto, Naohide. "Ferro- and antiferromagnetic interactions in face-sharing trioctahedral Ni^{II}Mn^{II}Ni^{II} and Ni^{II}Fe^{III}Ni^{II} complexes with the same 1-5/2-1 spin system." *J. Chem. Soc.; Chem. Comm.*, (2006), 1950-1952.
137. Nunzi, Francesca; Sgamellotti, Antonio; **Re, Nazzareno** "A density functional study of the dissociative adsorption of aromatic molecules on the Si(100) surface: on the way from benzene to larger polycyclic hydrocarbons" *J. Phys. Chem. C*, **2007**, *111*, 1392-1401.
138. Aschi Massimiliano; Besker Neva; Re Nazzareno; Pochetti Giorgio; Coletti Cecilia; Gallina Carlo; Mazza Fernando "Stereoselectivity by enantiomeric inhibitors of matrix metalloproteinase-8: new insights from molecular dynamics simulations" *J. Med. Chem.* **2007**, *50*, 211-218.
139. Hamamatsu Takefumi, Yabe Kazuya, Towatari Masaaki, Matsumoto, Naohide, **Re, Nazzareno**, Pochaba, Andrzej, Mrozinski, Jerzy, "Synthesis and magnetic property of copper(II)-lanthanide(III) complexes [{Cu(II)LLn(III)(o-van)(CH₃COO)(MeOH)}₂] 2H₂O (Ln(III) = Gd-III, Tb-III, and Dy-III; H₃L=1-(2-hydroxybenzamido)-2-(2-hydroxy-3-methoxybenzylideneamino)ethane; o-van=3-methoxysalicylaldehydato)" *Bulletin of the Chemical Society of Japan*, **2007**, *3*, 523-529.
140. Cerofolini Gianfranco, Marrone Alessandro, **Re Nazzareno** "Local and non-local properties controlling the strength of Bronsted acids and bases" *Journal of Molecular Structure (THEOCHEM)*, **2007**, *810*, 121-128.
141. Hamamatsu Takefumi, Yabe Kazuya, Towatari Masaaki, Osa Shutaro, Matsumoto Naohide, Re, Nazzareno, Pochaba, Andrzej, Mrozinski, Jerzy, Gallani Jean-Luis, Barla Alessandro, Imperia Paolo, Paulsen Carley, Kappler, Jean Paul "Magnetic interactions in Cu-II-Ln(III) cyclic tetranuclear complexes: Is it possible to explain the occurrence of SMM behavior in Cu-II-Tb-III and Cu-II-Dy-III complexes?" *Inorganic Chemistry*, **2007**, *46*, 4458-4468.
142. Besker Neva, Coletti Cecilia, Marrone Alessandro, **Re Nazzareno** "Binding of antitumor ruthenium complexes to DNA and proteins: A theoretical approach" *Journal of Physical Chemistry B*, **2007**, 9955-9964.

143. De Angelis Filippo, Sgamellotti Antonio, **Re Nazzareno** "Full quantum mechanical investigation of the unimolecular versus bimolecular acetylene to vinylidene rearrangement in the prototype trans-Cl-Rh(Pi-Pr-3)(2) complex" *Organometallics*, **2007**, 26, 5285-5288.
144. Yabe Kazuya, Maruno Yuji, Towatari Masaaki, Hamamatsu Takefumi, Matsumoto, Naohide, Re, Nazzareno, Pochaba, Andrzej, Mrozinski, Jerzy, "One-dimensional structure consisting of pin-wheel CU4Gd core and Na+ as connector" *Chemistry Letters*, **2007**, 36, 1452-1453.
145. Marrone, Alessandro; Re, Nazzareno; Romeo, Raffaello "Dissociative Route to C-H Bond Activation: DFT Study of Ligand Cyclometalation in a Platinum(II) Complex" *Organometallics* **2008**, 27, 2215-2222.
146. Yamaguchi, T.; Sunatsuki, Y.; Ishida, H.; Kojima, M.; Akashi, H.; Re, N.; Matsumoto, N.; Pochaba, A.; Mroziński, J. "Synthesis, Structures, and Magnetic Properties of Face-Sharing Heterodinuclear Ni(II)-Ln(III) (Ln = Eu, Gd, Tb, Dy) Complexes" *Inorg. Chem.* **2008**, 47, 5736-5745.
147. Gallo, Vito; Latronico, Mario; Mastrorilli, Piero; Nobile, F. Cosimo; Polini, Flavia; Re, Nazzareno; Englert, Ulli "Reactivity of a Phosphinito-Bridged Pt^I-Pt^I Complex with Nucleophiles: Substitution versus Addition" *Inorg. Chem.* **2008**, 47, 4785-4795.
148. Nunzi, Francesca; Sgamellotti, Antonio; Coletti, Cecilia; Re, Nazzareno "Adsorption and Interfacial Chemistry of Pentacene on the Clean Si(100) Surface: A Density Functional Study" *J. Phys. Chem. C.* **2008**, 112, 6033-6048.
149. Besker, Neva; Coletti, Cecilia; Marrone, Alessandro; Re, Nazzareno "Aqueation of the Ruthenium-Based Anticancer Drug NAMI-A: A Density Functional Study" *J. Phys. Chem. B.* **2008**; 112, 3871-3875.
150. Yamaguchi, Tomoka; Sunatsuki, Yukinari; Ishida, Hiroyuki; Kojima, Masaaki; Akashi, Haruo; Re, Nazzareno; Matsumoto, Naohide; Pochaba, Andrzej; Mrozinski, Jerzy. "Synthesis, structures, and magnetic properties of doubly face-sharing heterotrinary NiII-LnIII-NiII (Ln = Eu, Gd, Tb, and Dy) complexes" *Bulletin of the Chemical Society of Japan* **2008**, 81, 598-605.
151. Ammazalorso, Alessandra; Bettoni, Giancarlo; De Filippis, Barbara; Fantacuzzi, Marialuigia; Giampietro, Letizia; Giancrisofaro, Antonella; Maccallini, Cristina; Re, Nazzareno; Amoroso, Rosa; Coletti, Cecilia "Synthesis of 2-aryloxypropanoic acids analogues of clofibrilic acid and assignment of the absolute configuration by 1H NMR spectroscopy and DFT calculations" *Tetrahedron: Asymmetry* **2008**, 19, 989-997.
152. Latronico, Mario; Polini, Flavia; Gallo, Vito; Mastrorilli, Piero; Calmuschi-Cula, Beatrice; Englert, Ulli; Re, Nazzareno; Repo, Timo; Raisainen, Mina "Site Selectivity in the Protonation of a Phosphinito Bridged Pt^I-Pt^I Complex: a Combined NMR and Density-Functional Theory Mechanistic Study" *Inorg. Chem.* **2008**, 47, 9779-9796.
153. Angela Casini, Chiara Gabbiani, Francesca Sorrentino, Maria Pia Rigobello, Alberto Bindoli, Tilmann J. Geldbach, Alessandro Marrone, Nazzareno Re, Christian G. Hartinger, Paul J. Dyson and Luigi Messori "Emerging Protein Targets for Anticancer Metallodrugs: Inhibition of Thioredoxin Reductase and Cathepsin B by Antitumor Ruthenium(II)-Arene Compounds" *J. Med. Chem.*, **2008**, 51, 6773-6781.
154. Cecilia Coletti Nazzareno Re, "High Level Theoretical Study of Benzene-Halide Adducts: The Importance of C-H-Anion Hydrogen Bonding" *J. Phys. Chem. A*, **2009**, 113, 1578-1585.
155. Cristina Maccallini, Antonia Patruno, Neva Besker, Jamila Isabella Ali, Alessandra Ammazalorso, Barbara De Filippis, Sara Franceschelli, Letizia Giampietro, Mirko Pesce, Marcella Reale, Maria L. Tricca, Nazzareno Re, Mario Felaco and Rosa Amoroso "Synthesis, Biological Evaluation, and Docking Studies of N-Substituted Acetamidines as Selective Inhibitors of Inducible Nitric Oxide Synthase" *J. Med. Chem.*, **2009**, 52, 1481-1485.
156. Margarita Alberti, Antonio Aguilar, Josep M. Lucas, Fernando Pirani, Cecilia Coletti Nazzareno Re, "Atom-bond Pairwise Additive representation for Halide-Benzene Potential Energy Surfaces: an ab initio Validation Study" *J. Phys. Chem. A*, **2009**, 113, 14606-14614.

157. Francesco Creati, Cecilia Coletti, Nazzareno Re, "Density functional study of butadiyne to butatrienyliene isomerization in $[\text{Ru}(\text{HCCCCH})(\text{Pme}_3)_2(\text{Cp}^*)]$ " *Organometallics*, **2009**, *28*, 6603-6616.
158. Marrone Alessandro, Renzetti Andrea, De Maria Paolo, Gérard S., Sapi J., Fontana A., Re N. "Condensation of β -diester titanium enolates with carbonyl substrates: A combined DFT and experimental investigation" *Chemistry - A Eur. J.* **2009**, *15*, 11537-11550.
159. Fantauzzi, S., Gallo, E., Caselli, A., Piangiolino, C., Ragaini, F., Re, N., Cenini, S. "Rearrangement of N-Aryl-2-vinylaziridines to benzoazepines and dihydropyrroles: A synthetic and theoretical study" *Chemistry - A Eur. J.* **2009**, *15*, 1241-1251.
160. Yoshida, T., Towatari, M., Sato, T., Matsumoto, N., Re, N., Mrozinski, J. "A ferromagnetic chain of imidazolato-bridged one-dimensional copper(ii) complex" *Bulletin of the Chemical Society of Japan* **2009**, *82*, 467-473.
161. Hamamatsu T., Matsumoto N., Re N., Mrozinski J. "Chiral ferromagnetic chain of copper(II)-Gadolinium(III) complex" *Chemistry Letters* **2009**, *38*, 762-763.
162. Coletti C., Re N., Scuderi D., Maitre P., Chiavarino B., Fornarini S., Lanucara F., Sinha, R.K., Crestoni M.E. "IRMPD spectroscopy of protonated S-nitrosocaptopril, a biologically active, synthetic amino acid" *Physical Chemistry Chemical Physics* **2010**, *12*, 13455-13467.
163. Maccallini, C., Patruno, A., Lannutti, F., Ammazalorso, A., De Filippis, B., Fantacuzzi, M., Franceschelli, S., Giampietro, L., Masella, S., Felaco, M., Re, N., Amoroso, R. "N-Substituted acetamidines and 2-methylimidazole derivatives as selective inhibitors of neuronal nitric oxide synthase" *Bioorganic and Medicinal Chemistry Letters* **2010**, *20*, 6495-6499
164. Casini, A., Edafe, F., Erlandsson, M., Gonsalvi, L., Ciancetta, A., Re, N., Ienco, A., Messori, L., Peruzzini, M., Dyson, P.J. "Rationalization of the inhibition activity of structurally related organometallic compounds against the drug target cathepsin B by DFT" *Dalton Transactions* **2010**, *39*, 5556-5563.
165. Pochetti, G., Mitro, N., Lavecchia, A., Gilardi, F., Besker, N., Scotti, E., Aschi, M., Re, N., Fracchiolla, G., Laghezza, A., Tortorella, P., Montanari, R., Novellino, E., Mazza, F., Crestani, M., Loiodice, F. "Structural insight into peroxisome proliferator-activated receptor γ binding of two ureidofibrate-like enantiomers by molecular dynamics, cofactor interaction analysis, and site-directed mutagenesis" *Journal of Medicinal Chemistry* **2010**, *53*, 4354-4366.
166. Mastroilli, P., Latronico, M., Gallo, V., Polini, F., Re, N., Marrone, A., Gobetto, R., Ellena, S. "Facile activation of dihydrogen by a phosphinito-bridged Pt(II)-Pt(II) complex" *Journal of the American Chemical Society* **2010**, *132*, 4752-4765.
167. Maruno, Y., Yabe, K., Hagiwara, H., Fujinami, T., Matsumoto, N., Re, N., Mrozinski, J. "Cyclic and linear structures constructed by ionic bonds between alkali ion and pinwheel pentanuclear $[\text{GdIII}(\text{CuII})_4]$ core of $\text{M}[\text{GdIII}(\text{CuII})_4]$ ($\text{M}^+ = \text{Na}^+$, K^+ , and Cs^+ ; $\text{H}_3\text{L} = \text{N}-(4\text{-methyl-6-oxo-3-azahept-4-enyl)oxamic acid}$)" *Bulletin of the Chemical Society of Japan* **2010**, *83*, 1511-1517
168. Coletti, C., Gonsalvi, L., Guerriero, A., Marvelli, L., Peruzzini, M., Reginato, G., Re, N. "Rhenium allenylidenes and their reactivity toward phosphines: A theoretical study" *Organometallics* **2010**, *29*, 5982-5993
169. Shimogori, Y., Hamamatsu, T., Fujinami, T., Hagiwara, H., Matsumoto, N., Re, N., Mrozinski, J., Ishikawa, Y., Igashira-Kamiyama, A., Konno, T. "A linear $\text{CuII-GdIII-CuII-GdIII}$ complex derived from the assembly reaction of $[\text{NaCuIIH}_3\text{Ldpn}(\text{meso})]$ and $[\text{GdIII}(\text{thd})_3(\text{H}_2\text{O})_2]$ ($\text{H}_3\text{L} = \text{meso-1,2-diphenyl-1-(2-oxybenzamido)-2-(2-oxy-3-ethoxybenzylideneamino)ethane}$ and $\text{Hthd} = 2,2,6,6\text{-tetra-methyl-3,5-heptanedione}$)" *Polyhedron* **2011**, *30*, 1127-1133.
170. Ciancetta, A., Coletti, C., Marrone, A., Re, N. "Activation of carboplatin by chloride ions: A theoretical investigation" *Theoretical Chemistry Accounts* **2011**, *129*, 757-769.

171. Fantacuzzi, M., Maccallini, C., Lannutti, F., Patruno, A., Masella, S., Pesce, M., Speranza, L., (...), Amoroso, R. "Selective Inhibition of iNOS by Benzyl- and Dibenzyl Derivatives of N-(3-Aminobenzyl)acetamidine" *ChemMedChem* **2011**, 6, 1203-1206.
172. Latronico, M., Mastroilli, P., Gallo, V., Dell'Anna, M.M., Creati, F., Re, N., Englert, U. "Hyrido phosphanido bridged polynuclear complexes obtained by protonation of a phosphinito bridged Pt(I) complex with HBF₄ and HF" *Inorganic Chemistry* **2011**, 50, 3539-3558.
173. Lannutti F., Marrone, A., Re N. "Prediction of the PPAR α agonism of fibrates by combined MM-docking approaches" *Journal of Molecular Graphics and Modelling* **2011**, 29, 865-875.
174. Coletti, C., Re, N. "High level theoretical study of binding and of the potential energy surface in benzene-hydride system" *Chemical Physics* **2012**, 398, 168-175.
175. Re, N., Coletti, C., Marrone, A. "Metal complexes containing allenylidenes and higher cumulenylidenes ligands: a theoretical perspective" *Accounts of Chemical Research*, **2012**, 45, 139-149.
176. Lannutti, F., Marrone, A., Re, N., "Binding of GSH conjugates to d-GST: A cross-docking approach" *Journal of Molecular Graphics and Modelling*, **2012**, 32, 9-18.
177. Coletti, C., Gonsalvi, L., Guerriero, A., Marvelli, L., Peruzzini, M., Reginato, G., **Re, N.**, "Electron-poor rhenium allenylidenes and their reactivity toward phosphines: A combined experimental and theoretical study", *Organometallics*, **2012**, 31, 57-69.
178. Coletti, C., **Re, N.**, "Performance of DFT and MP2 approaches for geometry of rhenium allenylidenes complexes and the thermodynamics of phosphines addition", *Lecture Notes in Computer Science* (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics), 2012, 7333 LNCS PART 1, 738-751.
179. Sorrentino, S., Bucciarelli, T., Corsaro, A., Tosatto, A., Thellung, S., Villa, V., Schinina, M.E., Maras, B., Galeno, R., Scotti, L., Creati, F., Marrone, A., Re, N., Aceto, A., Florio, T., Mazzanti, M., "Calcium binding promotes prion protein fragment 90-231 conformational change toward a membrane destabilizing and cytotoxic structure", *PLoS ONE*, **2012**, 7, e38314.
180. Martins, A.P., Marrone, A., Ciancetta, A., Cobo, A.G., Echevarr a, M., Moura, T.F., Re, N., Casini, A., Soveral, G., "Targeting aquaporin function: Potent inhibition of aquaglyceroporin-3 by a gold-based compound", *PLoS ONE*, **2012**, 7, 5, e37435.
181. Tamboli, V.F., **Re, N.**, Coletti, C., Defant, A., Mancini, I., Tosi, P., "A joint experimental and theoretical investigation on the oxidative coupling of resveratrol induced by copper and iron ions", *International Journal of Mass Spectrometry*, **2012**, 319-320, 55-63.
182. Sakamoto, S., Yamauchi, S., Hagiwara, H., (...), Sunatsuki, Y., Re, N., "Carbonate-bridged tetranuclear Ni^{II}₂Gd^{III}₂ complex generated by atmospheric CO₂ fixation", *Inorganic Chemistry Communications*, 2012, 26, 20-23.
183. Ciancetta, A., Coletti, C., Marrone, A., Re, N., "Activation of carboplatin by carbonate: A theoretical investigation", *Dalton Transactions*, **2012**, 41, 12960-12969.
184. Todisco, S., Gallo, V., Mastroilli, P., (...), Creati, F., Braunstein, P., "Pt-Mo and Pt-W mixed-metal clusters with chelating or bridging diphosphine Short-Bite Ligands (Ph₂P)₂NH and (Ph₂P)₂N(CH₂)₉CH₃: A combined synthetic and theoretical study", *Inorganic Chemistry*, **2012**, 51, 11549-11561.
185. De Petris, A., Ciavardini, A., Coletti, C., (...), Crestoni, M.E., Fornarini, S., "Vibrational signatures of the naked aqua complexes from platinum(II) anticancer drugs", *Journal of Physical Chemistry Letters*, **2013**, 4, 3631-3635.
186. Ehama, K., Ohmichi, Y., Sakamoto, S., (...), Tsuchimoto, M., Re, N., "Synthesis, structure, luminescent, and magnetic properties of carbonate-bridged ZnII 2LnIII 2 complexes [(μ -4-CO₃)₂{ZnII N'-Bis(3-ethoxy-2-oxybenzylidene)-1,3-propanediaminato}]", *Inorganic Chemistry*, **2013**, 52, 12828-12841.

187. Martins, A.P., Ciancetta, A., deAlmeida, A., (...), Soveral, G., Casini, A., "Aquaporin inhibition by gold(III) compounds: New insights", *ChemMedChem*, **2013**, *8*, 1086-1092.
188. Sakamoto, S., Fujinami, T., Nishi, K., (...), Sunatsuki, Y., Re, N., "Carbonato-bridged NiII₂LnIII₂ (LnIII = GdIII, TbIII, DyIII) complexes generated by atmospheric CO₂ fixation and their single-molecule-magnet behavior: [(4-CO₃)₂{NiII(3-MeOsaltn)(MeOH or H₂O)LnIII(NO₃)₂solvent [3-MeOsaltn = N, N-Bis(3-methoxy-2-oxybenzylidene)-1,3-propanediaminato]}", *Inorganic Chemistry*, **2013**, *52*, 7218-7229.
189. Towatari, M., Nishi, K., Fujinami, T., (...), Re, N., Mrozinski, J., "Syntheses, structures, and magnetic properties of acetato- and diphenolato-bridged 3d-4f binuclear complexes [M(3-MeOsaltn)(MeOH)_x(ac)Ln(hfac)₂](M = ZnII, CuII, NiII, CoII; Ln = LaIII, GdIII, TbIII, DyIII; 3-MeOsaltn = N, N-Bis(3-methoxy-2-oxybenzylidene)-1,3-propanediaminato; Ac = Acetato; Hfac = Hexafluoroacetylacetonato; X = 0 or 1)", *Inorganic Chemistry*, **2013**, *52*, 6160-6178.
190. Barone, C.R., Coletti, C., McQuitty, R.J., (...), Sadler, P.J., White, F.J., "Photo-isomerisation of alkenyl complexes of platinum(ii): Structural, spectroscopic, kinetic and computational investigations", *Dalton Transactions*, **2013**, *42*, 6840-6851.
191. Siehl, H.-U., Brixner, S., Coletti, C., (...), De Petris, A., Fornarini, S., "Isomeric C₅H₁₁Si⁺ ions from the trimethylsilylation of acetylene: An experimental and theoretical study", *International Journal of Mass Spectrometry*, **2013**, *334*, 58-66.
192. Lannutti, F., Marrone, A., Re, N., "Estimation of the PPAR α agonism of fibrates by a combined MM-docking approach" *Methods in Molecular Biology*, **2013**, *952*, 229-235.
193. Shintoyo, S., Murakami, K., Fujinami, T., (...), Coletti, C., Re, N., "Crystal field splitting of the ground state of terbium(III) and dysprosium(III) complexes with a triimidazolyl tripod ligand and an acetate determined by magnetic analysis and luminescence", *Inorganic Chemistry*, **2014**, *53*, 10359-10369.
194. Yamauchi, S., Fujinami, T., Matsumoto, N., (...), Coletti, C., Re, N., "Synthesis, structure, luminescence, and magnetic properties of a single-ion magnet " mer "-[tris(N-(imidazol-4-yl)-methylidene)-dl-phenylalaninato]terbium(III) and related " fac "-Dl-alaninato derivative", *Inorganic Chemistry*, **2014**, *53*, 5961-5971.
195. Inoue, M., Suzuki, T., Sunatsuki, Y., Fuyuhiko, A., Re, N., "Chiral incomplete-cubane-type MnIII 3O₄ clusters containing a μ -3-methoxido or hydroxido", *Chemistry Letters*, **2014**, *43*, 784-786.
196. Maccallini, C., Montagnani, M., Paciotti, R., Re, N., (...), Pandolfi, A., Amoroso, R., "Acetamide-Based Nitric Oxide Synthase Inhibitors: Synthesis, Docking, and Biological Studies" *ACS Medicinal Chemistry Letters*, **2015**, *6*, 635-640.
197. Todisco, S., Mastroilli, P., Latronico, M., Re, N., (...), Creati, F., Braunstein, P., "Sulfur-Assisted Phenyl Migration from Phosphorus to Platinum in PtW₂ and PtMo₂ Clusters Containing Thioether-Functionalized Short-Bite Ligands of the Bis(diphenylphosphanyl)amine-Type", *Inorganic Chemistry*, **2015**, *54*, 4777-4798.
198. De Petris, A., Chiavarino, B., Crestoni, M.E., (...), Re, N., Fornarini, S., "Exploring the conformational variability in the heme b propionic acid side chains through the effect of a biological probe: A study of the isolated ions" *Journal of Physical Chemistry A*, **2015**, *119*, 1919-1929.
199. Storchi, L., Paciotti, R., Re, N., Marrone, A., "Investigation of the molecular similarity in closely related protein systems: The PrP case study", *Proteins: Structure, Function and Bioinformatics*, **2015**, *83*, 1751-1765.
200. Renzetti, A., Marrone, A., Gérard, S., (...), Re, N., Fontana, A. "TiCl₄-promoted condensation of methyl acetoacetate, isobutyraldehyde, and indole: A theoretical and experimental study" *Physical Chemistry Chemical Physics*, **2015**, *17*, 8964-8972.
201. Re, N., Fantacuzzi, M., Maccallini, C., Paciotti, R., Amoroso, R. "Recent developments of amidine-like compounds as selective NOS inhibitors", *Current Enzyme Inhibition* **2016**, *12*, 30-39.

202. Corinti, D., Coletti, C., Re, N., (...), Crestoni, M.E., Fornarini, S. "Cisplatin Binding to Biological Ligands Revealed at the Encounter Complex Level by IR Action Spectroscopy" *Chemistry - A European Journal*, **2016**, 22, 3794-3803.
203. Hamada, D., Fujinami, T., Yamauchi, S., (...), Coletti, C., Re, N. "Luminescent DyIII single ion magnets with same N6O3 donor atoms but different donor atom arrangements, 'fac'-[DyIII(HLDL-ala)3]•8H2O and 'mer'-[DyIII(HLDL-phe)3]•7H2O", *Polyhedron*, 2016, 109, 120-128.
204. Marrone, A., Re, N., Storchi, L., "The effects of Ca²⁺ concentration and E200K mutation on the aggregation propensity of PrPC: A computational study", *PLoS ONE*, **2016**, 11, e0168039.
205. Graziani, V., Coletti, C., Marrone, A., Re, N. "Activation and Reactivity of a Bispidine Analogue of Cisplatin: A Theoretical Investigation", *Journal of Physical Chemistry A*, **2016**, 120, 5175-5186.
206. Ueno, T., Fujinami, T., Matsumoto, N., (...), Ishida, T., Sunatsuki, Y. "Circular and Chainlike Copper(II)-Lanthanide(III) Complexes Generated by Assembly Reactions of Racemic and Chiral Copper(II) Cross-Linking Ligand Complexes with LnIII(NO₃)₃•6H₂O (LnIII = GdIII, TbIII, DyIII)", *Inorganic Chemistry*, **2017**, 56, 1679-1695.
207. Corinti, D., De Petris, A., Coletti, C., (...), Crestoni, M.E., Fornarini, S. "Cisplatin Primary Complex with L-Histidine Target Revealed by IR Multiple Photon Dissociation (IRMPD) Spectroscopy", *ChemPhysChem.*, **2017**, 18, 318-325.
208. Corinti, D., Coletti, C., Re, N., (...), Crestoni, M.E., Fornarini, S. "Hydrolysis of cis- and transplatin: structure and reactivity of the aqua complexes in a solvent free environment", *RSC Advances*, **2017**, 7, 15877-15884.
209. Graziani, V., Marrone, A., Re, N., (...), Platts, J.A., Casini, A. "A Multi-Level Theoretical Study to Disclose the Binding Mechanisms of Gold(III)-Bipyridyl Compounds as Selective Aquaglyceroporin Inhibitors" *Chemistry - A European Journal* **2017**, 23, 13802-13813.
210. Paciotti, R., Corinti, D., De Petris, A., Re, N. (...), Elisa Crestoni, M., Fornarini, S. "Cisplatin and transplatin interaction with methionine: Bonding motifs assayed by vibrational spectroscopy in the isolated ionic complexes" *Physical Chemistry Chemical Physics* **2017**, 19, 26697-26707.
211. Tolbatov, I.; Coletti, Cecilia; Marrone, Alessandro; Re, Nazzareno "Insight into the Electrochemical Reduction Mechanism of Pt(IV) Anticancer Complexes" *Inorganic Chemistry*, **2018**, 57, 3411-3419.
212. Maccallini, C.; Di Matteo, M.; Gallorini, M.; (...) Re, N.; Pandolfi, A.; Cataldi, A.; Amoroso, R. "Discovery of N-{3-[(ethanimidoylamino)methyl]benzyl}-L-prolinamide dihydrochloride: A new potent and selective inhibitor of the inducible nitric oxide synthase as a promising agent for the therapy of malignant glioma" *European Journal Of Medicinal Chemistry* **2018**, 152, 53-64.
213. Paciotti, R., Tolbatov, I., Graziani, V., (...), Re, N., Coletti, C., "Insights on the activity of platinum-based anticancer complexes through computational methods", *AIP Conference Proceedings*, **2018**, 2040, 020019.
214. Paciotti, R., Tolbatov, I., Marrone, A., (...), Re, N., Coletti, C., "Computational investigations of bioinorganic complexes: The case of calcium, gold and platinum ions" *AIP Conference Proceedings*, **2019**, 2186, 030011.
215. Tolbatov, I., Re, N., Coletti, C., Marrone, A. "An Insight on the Gold(I) Affinity of golB Protein via Multilevel Computational Approaches", *Inorganic Chemistry*, **2019**, 58, 11091-11099. 2
216. Coppola, C.M., Tolbatov, I., Tranca, I.C., (...), Fernandez-Villace, V., Longo, J., "A database approach for materials selection for hydrogen storage in aerospace technology", *Rendiconti Lincei*, **2019**, 90, 287-296.

217. Wenzel, M.N., Mósca, A.F., Graziani, V., (...), Soveral, G., Casini, A., "Insights into the Mechanisms of Aquaporin-3 Inhibition by Gold(III) Complexes: The Importance of Non-Coordinative Adduct Formation" *Inorganic Chemistry*, **2019**, 58, 2140-2148. 7
218. Tolbatov, I., Coletti, C., Marrone, A., Re, N., "Reactivity of gold(I) monocarbene complexes with protein targets: A theoretical study", *International Journal of Molecular Sciences*, **2019**, 20, 820.
219. Corinti, D., Coletti, C., Re, N., (...), Crestoni, M.E., Fornarini, S., "Short-lived intermediates (encounter complexes) in cisplatin ligand exchange elucidated by infrared ion spectroscopy", *International Journal of Mass Spectrometry*, **2019**, 435, 7-17.
220. Tolbatov, I., Re, N., Coletti, C., Marrone, A. Determinants of the Lead(II) Affinity in pbrR Protein: A Computational Study, *Inorganic Chemistry*, **2020**, 59, 790-800.
221. Corinti, D., Paciotti, R., Re, N., (...), Crestoni, M.E., Fornarini, S. "Binding motifs of cisplatin interaction with simple biomolecules and aminoacid targets probed by IR ion spectroscopy" *Pure and Applied Chemistry*, **2020**, 92, 3-13.