List of Publications of Pina ROMANIELLO (last update october 2021)

My scientific work has been published in 44 peer-reviewed articles, with more than 1000 citations. All publications are listed in the following.

1. *Scrutinizing GW-based methods using the Hubbard dimer*
   S. Di Sabatino, P.-F. Loos, and **P. Romaniello**
   Front. Chem. **9**, 865 (2021)

2. *Photoemission spectra from the Extended Koopman's Theorem, revisited*
   S. Di Sabatino, J. Koskelo, J. Prodhon, J.A. Berger, M. Caffarel, and **P. Romaniello**
   Front. Chem. **9**, 819 (2021)

3. *Time dependent reduced density matrix functional theory at strong correlation : insights from a two-site Anderson impurity model description*
   S. Di Sabatino, C. Verdozzi, and **P. Romaniello**
   Phys. Chem. Chem. Phys. **23**, 16730 (2021)

4. *Photoemission spectrum in paramagnetic FeO under pressure: towards an ab initio description*
   S. Di Sabatino, J. Koskelo, J.A. Berger and **P. Romaniello**
   Phys. Rev. Research **3**, 013172 (2021)

5. *Potential energy surfaces without unphysical discontinuities : the Coulomb-hole plus screened exchange approach*
   J.A. Berger, P.-F. Loos, and **P. Romaniello**
   J. Chem. Theory Comput. **17**, 191 (2021)

6. *Optical spectra of 2D monolayers from time-dependent density functional theory*
   S. Di Sabatino, J.A. Berger, and **P. Romaniello**
   Faraday Discussions, **224**, 467 (2020)

7. *Accurate optical spectra of solids from pure time-dependent density-functional theory*
   S. Cavo, J.A. Berger and **P. Romaniello**
   Phys. Rev. B **11**, 115109 (2020)

8. *Many-Body Effective Energy Theory: Photoemission at Strong Correlation*
   S. Di Sabatino, J.A. Berger and **P. Romaniello**
   J. Chem. Theory Comput. **15**, 5080 (2019)

9. *Unphysical Discontinuities in GW Methods*
   M. Véril, **P. Romaniello**, J. A. Berger, and Pierre-Franǫis Loos
   J. Chem. Theory Comput. **14**, 5220 (2018)

10. *Green functions and self-consistency: insights from the spherium model*
    Pierre-François Loos, **P. Romaniello**, and J. A. Berger
    J. Chem. Theory Comput. **14**, 3071(2018)

11. *Optical properties from time-dependent current-density- functional theory: the case of the alkali metals Na, K, Rb, and Cs*
    R. R. Ferrádas, J.A. Berger, and **P. Romaniello**
    Eur. Phys. J B 91, **119** (2018); Special issue in honor of Hardy Gross

12. *Many-body perturbation theory and non-perturbative approaches: the screened interaction as key ingredient*
    W. Tarantino, B. Mendoza **P. Romaniello**, J. A. Berger, and L. Reining
    J. Phys.: Condens. Matter **30**, 135602 (2018)

13. *Self-consistent Dyson equation and self-energy functionals : An analysis and illustration on the example of the Hubbard atom*
    W. Tarantino, **P. Romaniello**, J. A. Berger, and L. Reining
    Phys. Rev. B **96**, 045124 (2017)

14. *Optical properties of periodic systems within the current-current response framework: pitfalls and remedies*
D. Sangalli. J.A. Berger, C. Attaccalite, M. Gruening, and **P. Romaniello**
Phys. Rev. B **95**, 155203 (2017)

15. *Photoemission Spectra from Reduced Density Matrices: the Band Gap in Strongly Correlated Systems*
S. Di Sabatino, J.A. Berger, L. Reining, and **P. Romaniello**
Phys. Rev. B **94**, 155141 (2016)

16. *Gauge-Invariant Formulation of Circular Dichroism*
N. Raimbault, P. L. de Boeij, **P. Romaniello**, and J. A. Berger
J. Chem. Theory Comput. **12**, 3278 (2016)

17. *Unphysical and physical solutions in many-body theories: from weak to strong correlation*
A. Stan, **P. Romaniello**, S Rigamonti, L. Reining, and J.A. Berger
New J. Phys. **17**, 093045 (2015)

18. *Reduced Density-Matrix Functional Theory: correlation and spectroscopy*
S. Di Sabatino, J.A. Berger, L. Reining, and **P. Romaniello**
J. Chem. Phys. **143**, 024108 (2015)

19. *Towards time-dependent current-density-functional theory in the non-linear regime*
J. M. Escartín, M. Vincendon, **P. Romaniello**, P. M. Dinh, P.-G. Reinhard, and E. Suraud
J. Chem. Phys. **142**, 084118 (2015)

20. *Gauge-Invariant Calculation of Static and Dynamical Magnetic Properties from the Current Density*
N. Raimbault, P. L. de Boeij, **P. Romaniello**, and J. A. Berger
Phy. Rev. Lett. **114**, 066404 (2015)

21. *Solution to the many-body problem in one point*
J. A. Berger, **P. Romaniello**, F. Tandetzky, B. Mendoza, C. Brouder, and L. Reining
New J. Phys. **16**, 113025 (2014)

22. *Photoelectron spectra from full time dependent self-interaction correction*
M. Vincendon, P. M. Dinh, **P. Romaniello**, P.-G. Reinhard, and E. Suraud
EPJ D **67**, 97 (2013)

23. *Calculation of photoelectron spectra: A mean-field-based scheme*
P. M. Dinh, **P. Romaniello**, P.-G. Reinhard, and E. Suraud
Phys. Rev. A **87**, 032514 (2013)

24. *On transition rates in surface hopping*
J. M. Escartín, **P. Romaniello**, L. Stella, P.-G. Reinhard, and E. Suraud
J. Chem. Phys. **137**, 234113 (2012)

25. *Beyond the GW approximation: Combining correlation channels*
P. Romaniello, F. Bechstedt, and L. Reining
Phys. Rev. B **85** 155131 (2012)

26. *Approximations for many-body Green's functions: insights from the fundamental equations*
G. Lani, **P. Romaniello**, and L. Reining
New J. Phys. **14**, 013056 (2012)

27. *Valence Electron Photoemission Spectrum of Semiconductors: Ab Initio Description of Multiple Satellites*
M. Guzzo, G. Lani, F. Sottile, **P. Romaniello**, M. Gatti, J.J. Kas, J. J. Rehr, M. G. Silly, F. Sirotti, and L. Reining
Phys. Rev. Lett. **107**, 166401 (2011)

28. *Double excitations in correlated systems: a many-body approach*
D. Sangalli, **P. Romaniello**, G. Onida, and A. Marini
J. Chem. Phys. **134**, 034115, (2011)

29. *Nonlinear optical properties of Ni(Me_6pzS_2)MX (M=Ni, Pd, Pt; X=Me_2timdt, mnt)*
P. Romaniello, M. C. D'Andria, and F. Lelj
J. Phys. Chem. A **114**, 5838, (2010)

30. *The self-energy beyond GW: Local and nonlocal vertex corrections*
P. Romaniello, S. Guyot, and L. Reining
J. Chem. Phys. **131**, 154111 (2009)

31. *Double excitations in finite systems*
P. Romaniello, D. Sangalli, J. A. Berger, F. Sottile, L. Molinari, L. Reining, and G. Onida
J. Chem. Phys. **130**, 044108 (2009)

32. *Relativistic two-component formulation of time-dependent current-density functional theory: application to the linear response of solids*
P. Romaniello and P. L. de Boeij
J. Chem. Phys. **127**, 174111 (2007)

33. *Structural and new spectroscopic properties of neutral [M($dmit)_2$] (dmit= $C_3S_5^{2-}$, 1,3-dithiole-2-thione-4,5-dithiolate) and [M(H_2timdt)$_2$] (H_2timdt= $H_2C_3N_2S_3^{1-}$, monoanion of imidazolidine-2,4,5-trithione) complexes within the density functional approach*
P. Romaniello, F. Lelj, M. Arca, and F.A. Devillanova
Theor. Chem. Acc. **117**, 621 (2007)

34. *Performance of the Vignale-Kohn functional in the Linear response of Metals*
J.A. Berger, **P. Romaniello**, R. van Leeuwen, and P.L. de Boeij
Phys. Rev. B **74**, 245117 (2006)

35. *Optical properties of bcc transition metals in the range 0-40 eV*
P. Romaniello and P. L. de Boeij, F. Carbone and D. van der Marel
Phys. Rev. B **73**, 075115 (2006)

36. *The role of relativity in the optical response of gold within the time-dependent current-density-functional theory*
P. Romaniello and P. L. de Boeij
J. Chem. Phys. **122**, 164303 (2005)

37. *Time-dependent current-density-functional theory for the metallic response of solids*
P. Romaniello and P. L. de Boeij
Phys. Rev. B **71**, 155108 (2005)

38. *Effects of fluorine atoms on the optical nonlinear response of stilbene derivatives*
P. Romaniello and F. Lelj J. Fluor. Chem. **125**, 145 (2004)

39. *Ground and excited states of [M(H_2timdt)$_2$] neutral dithiolenes (M = Ni, Pd, Pt; H2timdt = monoanion of imidazolidine-2,4,5-trithione): description within TDDFT and scalar relativistic (ZORA) approaches*
P. Romaniello, M.C. Aragoni, M. Arca, T. Cassano, C. Denotti, F.A. Devillanova, F. Isaia, F. Lelj, V. Lippolis, and R. Tommasi J. Phys. Chem. A **107**, 9679 (2003)

40. *Limits in the second-order response of [M(H_2imXdt) (H_2imYdt)] neutral complexes (M=Ni, Pd, Pt; H_2imXdt=monoanion of imidazolidine-2-chalcogenone- 4,5-dithione; X = O, S, Se; Y = O, S, Se; X not equal Y): a pure theoretical study based on TD-DFT approach and ZORA formalism*
P. Romaniello and F. Lelj
J. Mol. Struct. (Theochem) **636**, 23 (2003)

41. *NIR dyes based on [M(R,R'timdt)$_2$] metal-dithiolenes: Additivity of M, R, and R' contributions to tune the NIR absorption (M = Ni, Pd, Pt; R,R'timdt = monoreduced form of disubstituted imidazolidine-2,4,5-trithione)*
M.C. Aragoni, M. Arca, T. Cassano, C. Denotti, F.A. Devillanova, R. Frau, F. Isaia, F. Lelj, V. Lippolis, L. Nitti, **P. Romaniello**, R. Tommasi, and G. Verani
Europ. J. Inorg. Chem. **10**, 1939 (2003)

42. *Optical non-linear properties of the [MXY] neutral mixed-ligand dithiolenes (M=Ni, Pd, Pt; X=R_2timdt, dmit, mnt; Y=R_2timdt, dmit, mnt; X=AY). The role of coordinated metal, substituents and of high lying excited states*
P. Romaniello and F. Lelj
Chem. Phys. Lett. **372**, 51 (2003)

43. *Picosecond absorption saturation dynamics in neutral [M(R,R ' timdt)$_2$] metal- dithiolenes*
T. Cassano, R. Tommasi, L. Nitti, M.C. Aragoni, M. Arca, C. Denotti , F.A. Devillanova, F. Isaia, V. Lippolis, F. Lelj, and **P. Romaniello**
J. Chem. Phys. **118**, 5995 (2003)

44. *Halogen bond in $(CH_3)_nX$ (X=N, P, n=3; X=S, n=2) and $(CH_3)_nXO$ (X=N, P, n=3; X=S, n=2) adducts with CF_3I. Structural and energy analysis including relativistic zero-order regular approximation approach in a density functional theory framework*
P. Romaniello and F. Lelj
J. Phys. Chem. A **106**, 9114 (2002)