

Publications Arjan Berger

1. *Unphysical Discontinuities in GW Methods*
M. V eril, P. Romaniello, J. A. Berger, and P.-F. Loos
Accepted in J. Chem. Theory Comput. (DOI: 10.1021/acs.jctc.8b00745); arXiv:1807.07480 (2018)
2. *Distributed gaussian orbitals for the description of electrons in an external potential*
L. Brooke, A. Diaz-Marquez, S. Evangelisti, T. Leininger, P.-F. Loos, N. Suaud, and J. A. Berger
J. Mol. Mod. 24, 216 (2018)
3. *Green Functions and Self-Consistency: Insights From the Spherium Model*
P.-F. Loos, P. Romaniello, and J. A. Berger
J. Chem. Theory Comput. 14, 3071 (2018)
4. *Optical properties from time-dependent current-density-functional theory: the case of the alkali metals Na, K, Rb, and Cs*
R. Ferrad as, J. A. Berger, and P. Romaniello
Eur. J. Phys. B 91, 119 (2018)
5. *Signatures of Wigner localization in one-dimensional systems*
A. Diaz-Marquez, S. Battaglia, G. L. Bendazzoli, S. Evangelisti, T. Leininger, and J. A. Berger
J. Chem. Phys. 148, 124103 (2018)
6. *Revisiting the origin of satellites in core level photoemission of transparent conducting oxides: the case of n-doped SnO₂*
F. Borgatti, J. A. Berger, D. C eolin, J.S. Zhou, J.J. Kas, M. Guzzo, C.F. McConville, F. Offi, G. Panaccione, A. Regoutz, D.J. Payne, J.-P. Rueff, O. Bierwagen, M.E. White, J.S. Speck, M. Gatti, and R.G. Egdell
Phys. Rev. B 97, 155102 (2018)
7. *Many-body perturbation theory and non-perturbative approaches: the screened interaction as key ingredient*
W. Tarantino, B. S. Mendoza, P. Romaniello, J. A. Berger, and L. Reining
J. Phys.: Cond. Matter. 30, 135602 (2018)
8. *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).
9. *Optical properties of periodic systems within the current-current response framework: Pitfalls and remedies.*
D. Sangalli, J. A. Berger, C. Attaccalite, M. Gr uning, and P. Romaniello
Phys. Rev. B **95**, 155203 (2017).
10. *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).
11. *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).
12. *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).
 13. *Fully parameter-free calculation of optical spectra for insulators, semiconductors and metals from a simple polarization functional.*
J. A. Berger
Phys. Rev. Lett. **115**, 137402 (2015).
 14. *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).
 15. *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
Phys. Rev. Lett. **114**, 066404 (2015).
 16. *Exact solution to the many-body problem in one point.*
J. A. Berger, P. Romaniello, F. Tandetzky, B. S. Mendoza, Ch. Brouder, and, L. Reining
New J. Phys. **16**, 113025 (2014).
 17. *A rational reduction of CI expansions: combining localized molecular orbitals and selected charge excitations.*
T. Krah, N. Ben Amor, D. Maynau, J. A. Berger, and V. Robert
J. Mol. Mod. **20**, 2240 (2014).
 18. *Efficient calculation of the polarizability: a simplified effective-energy technique.*
J. A. Berger, L. Reining, and F. Sottile
Eur. Phys. J. B, **85**, 236 (2012).
 19. *Efficient GW calculations for SnO₂, ZnO, and rubrene: the effective-energy technique.*
J. A. Berger, L. Reining, and F. Sottile
Phys. Rev. B **85**, 085126 (2012).
 20. *Ab initio calculations of electronic excitations: Collapsing spectral sums.*
J. A. Berger, L. Reining, and F. Sottile
Phys. Rev. B **82**, 041103(R) (2010).
 21. *Double excitations in finite systems.*
P. Romaniello, D. Sangalli, J. A. Berger, F. Sottile, L. Molinari, L. Reining, G. Onida, J.
J. Chem. Phys. **130**, 044108 (2009).
 22. *Analysis of the Vignale-Kohn current functional in the calculation of optical spectra.*
J. A. Berger, P. L. de Boeij, and R. van Leeuwen.
Phys. Rev. B **75**, 035116 (2007).

23. *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).
24. *A physical model for the longitudinal polarizabilities of polymer chains.*
J. A. Berger, P. L. de Boeij, and R. van Leeuwen.
J. Chem. Phys. **123**, 174910 (2005).
25. *Analysis of the viscoelastic coefficients in the Vignale-Kohn functional: The cases of one- and three-dimensional polyacetylene.*
J. A. Berger, P. L. de Boeij, and R. van Leeuwen.
Phys. Rev. B **71**, 155104 (2005).
26. *Size-scaling of the polarizability of tubular fullerenes investigated with time-dependent (current)-density-functional theory.*
M. van Faassen, L. Jensen, J. A. Berger, and P. L. de Boeij.
Chem. Phys. Lett. **395**, 274 (2004).
27. *Application of time-dependent current-density-functional theory to nonlocal exchange-correlation effects in polymers.*
M. van Faassen, P. L. de Boeij, R. van Leeuwen, J. A. Berger, and J. G. Snijders.
J. Chem. Phys. **118**, 1044 (2003).
28. *Ultranonlocality in time-dependent current-density-functional theory: Applications to conjugated polymers.*
M. van Faassen, P. L. de Boeij, R. van Leeuwen, J. A. Berger, and J. G. Snijders.
Phys. Rev. Lett. **88**, 186401 (2002).
29. *Current-density-functional theory for optical spectra: A successful polarization functional.*
P. L. de Boeij, F. Kootstra, J. A. Berger, R. van Leeuwen, and J. G. Snijders.
J. Chem. Phys. **115**, 1995 (2001).