Sivan Refaely-Abramson

List of publications

1. S. Refaely-Abramson, R. Baer and L. Kronik, “Fundamental and excitation gaps in molecules of relevance for organic photovoltaics from an optimally tuned range-separated hybrid functional”, *Phys. Rev. B* 84, 075144-1/8 (2011), **Editor's Choice**.
2. L. Kronik, T. Stein, S. Refaely-Abramson, and R. Baer, “Excitation gaps of finite-sized systems from optimally-tuned range-separated hybrid functionals”, *J. Chem. Theory Comput.* 8, 1515-1531 (2012).
3. S. Refaely-Abramson, S. Sharifzadeh, N. Govind, J. Autschbach, J. B. Neaton, R. Baer, and L. Kronik, “Quasiparticle spectra from a non-empirical optimally-tuned range separated hybrid density functional”, *Phys. Rev. Lett.* 109, 226405-1/6 (2012).
4. S. Refaely-Abramson, S. Sharifzadeh, Manish Jain, R. Baer, J. B. Neaton, and L. Kronik, “Gap renormalization of molecular crystals from density functional theory”, *Phys. Rev. B* 88, 081204-1/5(RC) (2013).
5. D. A. Egger, S. Weismann, S. Refaely-Abramson*, S. Sharifzadeh, M. Dauth, R. Baer, S. Kümmel, J. B. Neaton, E. Zojer, and L. Kronik, “Outer-valence electron spectra of prototypical aromatic heterocycles from an optimally-tuned range-separated hybrid functional”, *J. Chem. Theory Comput.* 10, 1934-1952 (2014).
6. I. Tamblyn, S. Refaely-Abramson, J. B. Neaton, and L. Kronik, “Simultaneous Determination of Structures, Vibrations, and Frontier Orbital Energies from a Self-Consistent Range-Separated Hybrid Functional”, *J. Phys. Chem. Lett.*, 5, 2734-2741 (2014).
7. D. Lüftner, S. Refaely-Abramson, M. Pachler, R. Resel, M. G. Ramsey, L. Kronik, and P. Puschnig, “Experimental and theoretical electronic structure of quinacridone”, *Phys. Rev. B* 90, 075204-1/6 (2014).
8. L. Sepunaru, S. Refaely-Abramson, R. Lovrincic, Y. Gavrilov, P. Agrawal, Y. Levy, L. Kronik, I. Pecht, M. Sheves, D. Cahen, "Electronic Transport via Homo-peptides: The Role of Side Chains and Secondary Structure", J. Am. Chem. Soc., 137, 9617–9626 (2015).
9. S. Refaely-Abramson, M. Jain, S. Sharifzadeh, J. B. Neaton, and L. Kronik, “Solid-state optical absorption from optimally tuned time-dependent range-separated hybrid density functional theory”, *Phys. Rev. B* 92, 081204(R) (2015).