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Materials by design: methodological developments in the calculation of excited-state properties[1]

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Density functional theory (DFT) is one of the main tools used in first principle simulations of materials; however several of the current approximations of exchange and correlation functionals do not provide the level of accuracy required for predictive calculations of excited state properties. The application to heterogeneous systems of more accurate post-DFT approaches such as Many-Body Perturbation Theory (MBPT) – for example to nanostructured, disordered, and defective materials – has been hindered by high computational costs. In this talk recent methodological developments in MBPT calculations will be discussed, as recently implemented in the open source code WEST [1], which efficiently exploits HPC architectures. Results using a formulation that does not require the explicit calculation of virtual states, nor the storage and inversion of large dielectric matrices will be presented; these results include quasi particle energies for systems with thousands of electrons and encompass the electronic structure of aqueous solutions, spin defects in insulators, and benchmarks for molecules and solids containing heavy elements. Simplifications of MBPT calculations based on the use of static response properties, such as dielectric-dependent hybrid functionals [2], will also be discussed.

[1] www.west-code.org; M. Govoni, and G. Galli, J. Chem. Theory Comput. 11, 2680 (2015)
[2] J.H. Skone, M. Govoni, and G. Galli, Phys. Rev. B 89, 195112 (2014)

[1]Work done in collaboration with Hosung Seo, Peter Scherpelz, Ikutaro Hamada, Jonathan Skone, Alex Gaiduk, T. Anh Pham, and Giulia Galli. Supported by DOE-BES.