Title: **Large Scale Many-Body Perturbation Theory Calculations: Methodological Developments, Data Collections, Validation and Applications**

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Abstract:
One of the main tools used in first principle simulations of materials is Density Functional Theory; however, several of the approximate exchange and correlation functionals do not provide the level of accuracy required for predictive calculations of excited state properties. The application to large systems of more accurate post-DFT approaches such as Many-Body Perturbation Theory (MBPT) -- for example to heterogeneous systems, 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 implemented in the open source code WEST [1]. Results using a formulation that does not require the explicit calculation of virtual states will be presented, e.g. for aqueous solutions and spin defects in insulators [2]. We will discuss online data collections which contain benchmarking results. Simplifications of MBPT calculations based on the use of static response properties, such as dielectric-dependent hybrid functionals [3], will also be presented. We will also briefly discuss the ongoing activities of the Midwest Integrated Center for Computational Materials (MICCoM).

[1] www.west-code.org; M. Govoni et al., J. Chem. Theory Comput. 11, 2680 (2015).
[2] A. Gaiduk et al., J. Am. Chem. Soc. Commun. 138, 6912 (2016); H. Seo et al., Sci. Rep. 6, 20803 (2016); P. Scherpelz et al., J. Chem. Theory Comput. 12, 3523 (2016).
[3] J.H. Skone et al., Phys. Rev. B 89, 195112 (2014); J.H. Skone et al., Phys. Rev. B 93, 235106 (2016); N. Brawand et al., Phys. Rev. X 6, 041002 (2016).