**Coupling first principles molecular dynamics and many body perturbation theory calculations**

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Discovery and design of materials and molecules require the ability to compute multiple properties and to carry out simulations at different length and time scales. We will present recent algorithmic developments aimed at coupling advanced sampling methods with first principles molecular dynamics (FPMD) [1] and the latter with many body perturbation (MBPT) theory calculations [2]. We will also discuss recent progress in hybrid density functionals used in FPMD, and as starting point for MBPT calculations [3].

[1] *Hierarchical Coupling of First Principles Molecular Dynamics with Advanced Sampling Methods*, Emre Sevgen, Federico Giberti, Hythem Sidky, Jonathan Whitmer, Giulia Galli, Francois Gygi and Juan de Pablo, J. Chem. Theory. Comp., 14(6), 2881-2888 (2018).

[2] *A Finite-field Approach for GW Calculations Beyond the Random Phase Approximation*, He Ma, Marco Govoni, Francois Gygi and Giulia Galli, J. Chem. Theory. Comp., 15 (1), 154-164 (2019); *Finite-field approach to solving the Bethe-Salpeter equation,* Ngoc Linh Nguyen, He Ma, Marco Govoni, Francois Gygi and Giulia Galli. Phys. Rev. Lett., Accepted (2019).

[3] *Dielectric dependent hybrid functionals for heterogeneous materials,* Huihuo Zheng, Marco Govoni, Giulia Galli 2019 (submitted): <https://arxiv.org/abs/1901.00824>.