

Towards Quantum Force Fields Using Quantum Charged Oscillators

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Quantum Charged (or Drude) Oscillators (QDOs) [1,2] offer a fundamental framework for future fully quantum atomistic force fields. In this talk, I will first review the concepts and theory behind coupled QDOs and the many-body dispersion (MBD) method [2,3] in particular. Then, I will demonstrate how the QDO/MBD framework is applicable to describe interatomic induction, dispersion and exchange interactions [4,5]. Finally, recent extensions to describe interatomic vdW potentials at all distances and even covalently-bonded dimers will be shown [6,7,8]. These results, taken together, elucidate the high promise of the coupled QDO framework as a fully quantum atomistic force field that can be developed as a community effort.

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