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**Stacking of conjugated oligomers and polymers in solution from first-principles** DAMIAN SCHERLIS, Materials Science and Engineering, MIT, JEAN-LUC FATTEBERT, FRANCOIS GYGI, CASC, Lawrence Livermore National Laboratory, NICOLA MARZARI, Materials Science and Engineering, MIT
— The elucidation of the intermolecular interactions between conjugated polymers and oligomers in the condensed phase is essential to understand and design organic semiconductors and electrically active polymers. The stacking of charged layers and the spatial arrangement of the chains are determining factors in charge transfer processes and in the electronic and optical properties of these materials. In this work we address these issues from first principles employing different electronic structure techniques in vacuum and in solution. In particular, we use a novel implementation of the Car-Parrinello method at the DFT level, which couples self-consistently the Kohn-Sham equations with the effect of a dielectric continuum. This methodology is contrasted with other well established, quantum chemistry solvation approaches, in the investigation of charged thiophene oligomers and polymers (and other related compounds) in different solvent fields. We assess the role of the dielectric in the stacking of the charged layers, and show how the balance between electrostatics and covalent forces is tilted by the environment, eventually leading to stable or unstable total interactions.

Damian Scherlis
Materials Science and Engineering, MIT

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