Charge Transport Characterization in 2D COFs

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Two-dimensional (2D) materials have attracted great attention owing to their unique physical and chemical properties and as well as their wide range of applications in electronics, sensing, energy storage and conversion. Among these materials, 2D covalent organic frameworks (COFs) are an emerging class of crystalline porous polymers with structural tunability and diversity [1]. Despite the intensive studies on 2D COFs, charge transport properties of most of these materials are still unknown. In particular, their relation to molecular building block properties is a great challenge due to the combinatorial nature of reticular chemistry. Herein, we investigate the structural and electronic properties of porphyrin-based 2D COFs using density functional theory (DFT)-based first-principles approaches [2,3]. We are modelling charge transport properties by combining the semi-classical Boltzmann transport theory [4] and deformation potential theory (DPT) for acoustic and optical phonons [5,6]. The results are bechmarked against state-of-the-art electron-phonon averaged (EPA) calculations [7].

References

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Figures

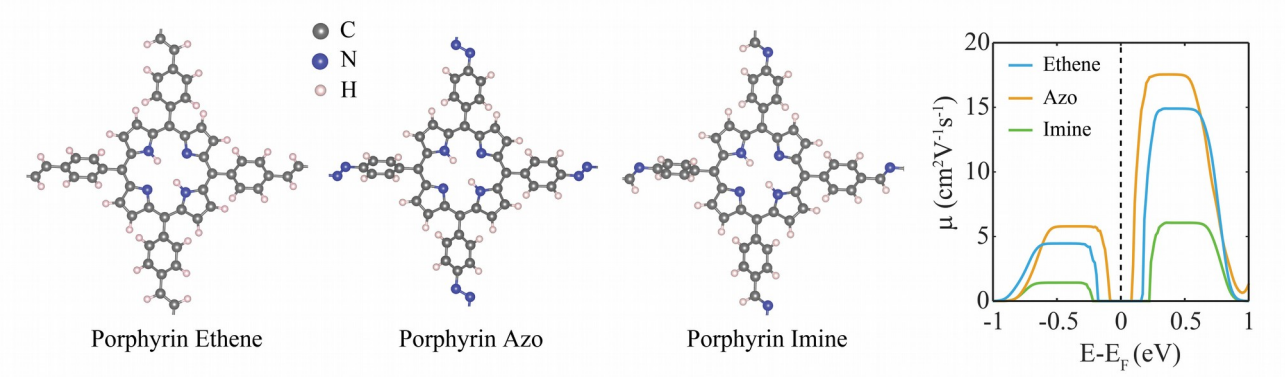

Figure 1: Top views of porphyrin-based structures and their calculated charge carrier mobilities within the acoustic DPT.