Predicting the electronic gap of single-layer 2D COFs from their molecular building-blocks

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Two-dimensional Covalent Organic Frameworks (2D COFs) have attracted a lot of interestdue to their large range of potential applications. Bottom-up engineering of theirmolecular building-blocks can lead to novel structures with fine-tuned physical andchemical properties. We have carried out a computational investigation of the electronicproperties of ~350 different 2D COFs with three- and four-arm cores. Four-arm coreswere modeled in 1D-polymer as alternating monomers of the respective 2D-polymer(COF) building units. Specifically, the electronic band structure of the periodic 1D- and2D-polymer, and the HOMO-LUMO difference of the respective molecular building-blockswere calculated. Considering a two-level system and using tight-binding approximation,an analytical model was derived to fit the conduction and valence bands. MachineLearning techniques were employed to find the weight of each variable and predict theelectronic band..

FIGURES

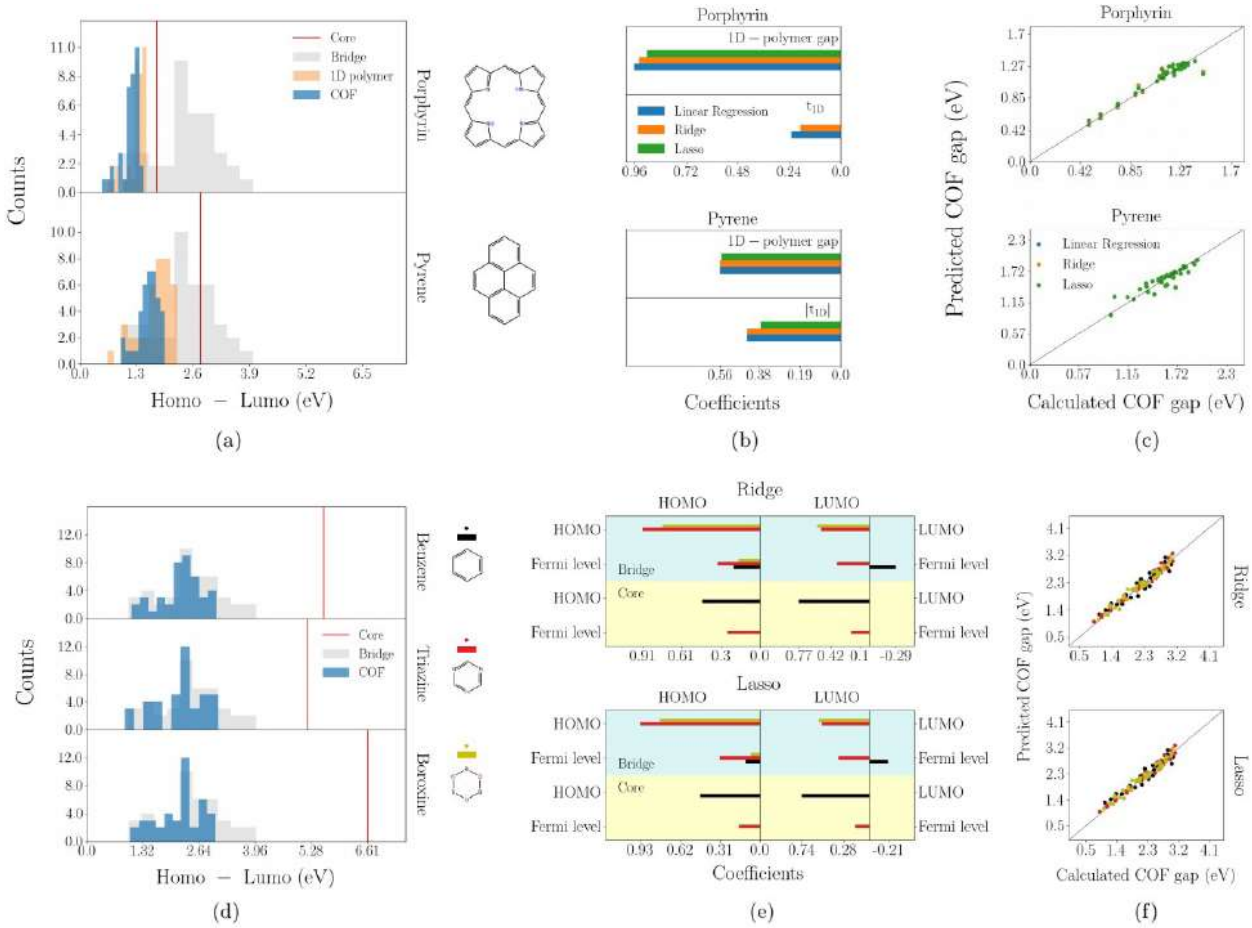

Figure 1: Figure 1: (a), (b) and (c) concern the four-arm cores, whereas (d), (e) and (f) the three arm-cores. (a) and (d) Histograms of HOMO-LUMO difference for the different bridge molecules, core, 1D-polymers and COFs. (b) and (e) Weights of the given variables to the algorithms. (c) and (f) Predicted vs caclulated gap.