Two-dimensional Covalent Organic Frameworks (2D COFs) have attracted a lot of interest due to their large range of potential applications. Bottom-up engineering of their molecular building-blocks can lead to novel structures with fine-tuned physical and chemical properties. We have carried out a computational investigation of the electronic properties of ~350 different 2D COFs with three- and four-arm cores. Four-arm cores were modeled in 1D-polymer as alternating monomers of the respective 2D-polymer(COF) building units. Specifically, the electronic band structure of the periodic 1D- and 2D-polymer, and the HOMO-LUMO difference of the respective molecular building-blocks were calculated. Considering a two-level system and using tight-binding approximation, an analytical model was derived to fit the conduction and valence bands. Machine Learning techniques were employed to find the weight of each variable and predict the electronic 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-polymer and COFs. (b) and (e) Weights of the given variables to the algorithms. (c) and (f) Predicted vs calculated gap.