Predicting the bulk modulus of single-layer 2D COFs from their molecular building-blocks properties

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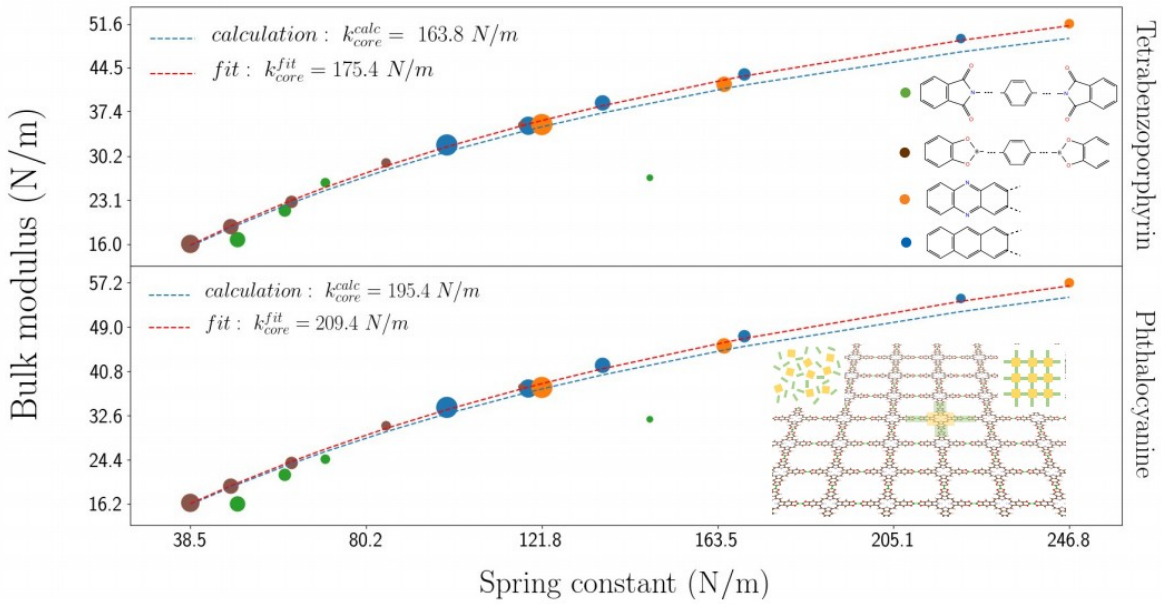
Two-dimensional Covalent Organic Frameworks (2D COFs) have attracted a lot of interest due to their large range of potential applications. Bottom-up engineering of their molecular building-blocks can lead to novel structures with fine-tuned physical and chemical properties. We have carried out a computational investigation of the elastic properties of different 2D COFs with square and hexagonal lattices. Specifically, the 2D bulk modulus and equivalent spring constants of the respective molecular building-blocks were calculated. Considering the material as a spring network, an analytical model for each topology was derived, which can be used to predict the 2D bulk modulus based on the properties of the monomeric units.

References

[1] A.Raptakis, A.Dianat, A.Croy and G.Cuniberti, Nanoscale, 2021, 13, 1077-1085



Figures

Figure 1: Correlation between spring constant and bulk modulus for the different cores with square lattice topology. The size of the circles for the structures is related to the number of the added benzene rings, while the color corresponds to the selected linker molecule as shown in the legend.