A Computational Study on Optical Absorption under High-pressure in Picene Crystal and Electron Transport through Porphyrin Based Single Molecular Device

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The electronic properties of picene crystal can be tuned by the application of high pressure up to 15 Gpa shown experimentally without losing its chemical stability [1]. In our calculation we optimized the geometry of the picene crystal [2] from 0-15 Gpa external pressure and calculated the optical band gap and volume contraction at each pressure using density functional theory (DFT). The calculated band gap as a function of applied pressure is in good agreement with experiment. In this poster we will also report the study of molecular conductance through a single molecular device made up with expanded porphyrin sandwiched between two gold metal electrodes. We used non-equlibrium Green's function (NEGF)-DFT based theory to calculate the conductance through molecular device[3]. In our calculation we took monomer, dimer, trimer and tetramer of fused porphyrin molecules to compare corresponding conductance with the length of the extended molecule.

References:

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2. De, A. et al. *Acta Cryst.* **1985**, *41*, 907-909.
3. Nitzan et al. *Science* **2003**, *300*, 1384-1389.