Polarons in Polyacetylene: Effects of Solvent Dielectric Constant

Frederick Bannier[1], Kamrun N. Keya[2] and Dmitri S. Kilin[1]

[1] Department of Chemistry and Biochemistry, North Dakota State University, Fargo, ND 58108, USA

[2]Department of Civil, Construction and Environmental Engineering, North Dakota State University, Fargo, ND 58108, USA

Polarons in conjugated polymers have been researched for decades, and further understanding of their formation/behavior may help to develop more efficient devices. One of the simplest materials demonstrating response of geometry and electronic structure to charge injection is cis-polyacetylene (cis-PA).[1] A range of cis-PA oligomers have been studied under condition of positive and negative charge injection. Injected portion of charge forms a continuous distribution that may be (a) off the geometrical center of the oligomer, even attracted to the edges and (b) may have a value of the width smaller than the one prompted by the size of the oligomer. These features of the charge distribution have been studied as a function of three conditions: (1) length of the oligomer, (2) sign of the injected charge, and (3) dielectric constant of the surrounding media. The exploration is performed by two approaches: DFT modeling as implemented in VASP software and by an iterative self-consistent model approach implemented via a MATLAB script. Through iterations, charge density and interatomic distances perturb each other. Compression of interatomic distances creates local minima in external potential, resulting in change of electron density localization pattern. These effects are slowed down in polar environments with higher dielectric constant. Similar patterns are observed in the model-simulated results and with DFT results for charged oligomers of cis-polyacetylene.

(1) Keya, K. N.; Xia, W.; Kilin, D. DFT simulation of conductivity of the p-type doped and charge-injected cis-polyacetylene. *Mol. Phys.* **2022**, e2110167. DOI: 10.1080/00268976.2022.2110167.