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Charge Induced Spin Polarization in Thiophene Oligomers AVADH SAXENA, Los Alamos National Lab, DONG HOU, JUNJIE QIU, SHI-JIE XIE, Shandong University — Charge induced spin polarization in organic small molecules is a key factor for spin transport and magnetic effects in related organic devices. We study the spin polarization in charged thiophene oligomer molecules by calculating the magnetic moment with density functional theory (DFT). We find that the emergence and variation of the net magnetic moment is related to both the amount of charge injected and the polymerization of the oligomer, i.e. the number of monomer units. Combined with model analysis, we conclude that the strong electron-electron (e-e) interaction and electron-lattice (e-l) interaction in organic materials are responsible for charge induced spin polarization in organic oligomers.

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