Significance of Structural Disorder For Charge Dynamics in θ-$(ET)_2X$ Materials

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θ-ET_2X materials are model two dimensional correlated electron systems known to exhibit a variety of electronic phenomena resulting from their frustrated inter-site Coulomb repulsions including charge ordered, glassy, and metallic states. The materials have drawn attention[1,2] in recent years particularly as to the phenomenon of charge vitrification and melting. In this study we consider the impact of structural disorder in the ethylene end groups (EEGs) of individual ET molecules for the charge dynamics in the bulk material. We computed electronic phase diagrams as a function of the inter-site coulomb repulsions and transfer integrals using a combination of Density Functional Theory (DFT) and Density Matrix Embedding Theory[3] (DMET). We find that the bulk electronic properties are significantly affected by the in-stack transfer integral, and that variation within this parameter caused by EEG disorder could be sufficient to induce local regions of metallic and crystallized charge states. This finding supports the hypothesis that EEG disorder can enhance charge glassiness, thus illustrating the importance of disorder in structural and electronic degrees of freedom in the physics of θ-$(ET)_2X$ materials.

References

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