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Multi-scale simulation on solid benzene HUA LIU, HENDRIK HEINZ — Solid Benzene is used in organic semiconductors for photovoltaics, which often include pi-conjugated systems. We use MD simulations method to explore the relationship between the structure and interaction energy of two kinds of solid benzene, with the Pbca and P21c crystallgraphic structures respectively. Simple relevant force fields (PCFF and CVFF) are examined with regard to their performance on the structure and energetics of benzene dimers and benzene crystals which serve as well characterized model systems. However, MD simulations cannot get the transport properties. So the combination of reliable classical atomistic simulations and quantum-mechanical methods is needed to understand the dynamics of charge transport and self-assembly processes involving pi-conjugated oligomers and polymers. As alternative and accurate models, we explore atomistic models with additional sites which represent the location of the pi electrons and are characterized by suitable charges and van-der-Waals parameters. With these parameters, it will be possible to reproduce the dimer geometries and energies, the crystal structure of solid benzene, as well as pi-stacking forces and free energies for similar systems.

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