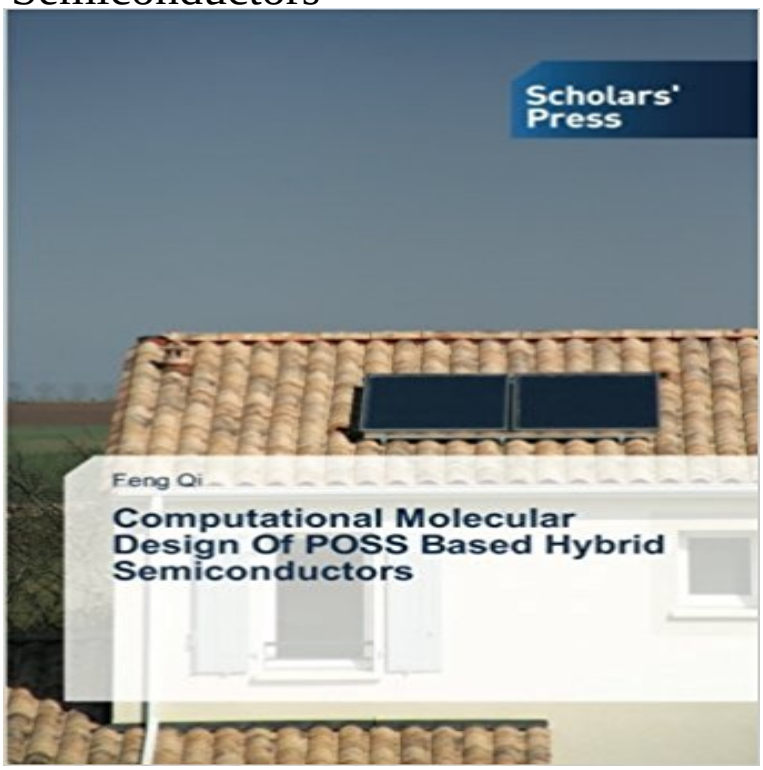
Computational Molecular Design Of POSS Based Hybrid Semiconductors



Cubic silsesquioxanes (T8 SQs), with the formula of [RSiO1.5]8, enable advanced materials design. A computational materials science framework, including ab initio density functional theory (DFT) calculations, molecular dynamics (MD), and Monte Carlo (MC) simulations, was developed to perform computational molecular design and crystal engineering of SQ based diacene-SQ and then octa(halogenphenyl)-SQ molecular systems. The goal was to identify novel molecular architectures, a priori, that exhibit targeted self-assembly behaviors and result in materials with improved electronic properties. First, existing force fields were evaluated for simulating cubic SQ systems. Next, targeting materials performance, a series of diacene-SQ molecules were designed and their crystal structures predicted by following the computational molecular design recipe. Computationally derived diacene-SQ crystals are predicted to exhibit advanced electronic properties. Finally, a series of new small-band gap octa(halogenphenyl)-SQ molecular systems were identified. These hybrid molecular crystals also feature other unique properties, such as solution processability, cubic molecular symmetry,etc.

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