Modelling Photoswitchable Organic-Graphene Hybrids

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Despite the recent advances in graphene-based electronics, several challenges still need to be addressed for real applications in electronics to flourish. Aiming at the design of a new generation of graphene-organic hybrid materials exhibiting multifunctional properties, we use classical molecular dynamics (MD) simulations to set up a model for the structural organization of 2D material-based light-responsive field-effect transistors incorporating photoresponsive self-assembled monolayers (SAM) between the 2D material and either metallic electrodes or gate dielectrics. The organization at both interfaces is of crucial importance for the description of charge injection/extraction/transport and assessing the overall device characteristics. Quantum-chemical validated force-field MD simulations are performed to characterize the SiO_2/SAM/graphene structure (tilt angle, structural disorder..) and model the photoswitching.