Charge transport in photoswitchable organic-graphene hybrids

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Abstract

Photoswitchable self-assembled monolayers (SAMs) in contact with a conductive or semiconductive layer can be used to remotely trigger changes in electrical current using light. In this study[1], we apply full-atomistic simulations to assess the changes in electronic structure and charge transport properties of a graphene sheet in contact with an amorphous silica dielectric decorated by an azobenzene SAM[2,3,4]. The simulations explicitly account for the structural and electrostatic disorder sourced by the dielectric, which turns out to be weakly affected by photoisomerization and spatially correlated over a length scale of 4–5 nm. Most interestingly, by combining large-scale density functional theory (DFT)-enriched tight-binding model with Kubo–Greenwood quantum transport calculations, we predict that the *trans-cis* isomerization should induce a shift in surface electrostatic potential by a few tenths of a volt, accompanied by a variation in conductivity by a factor of about three[1].

References

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Figures

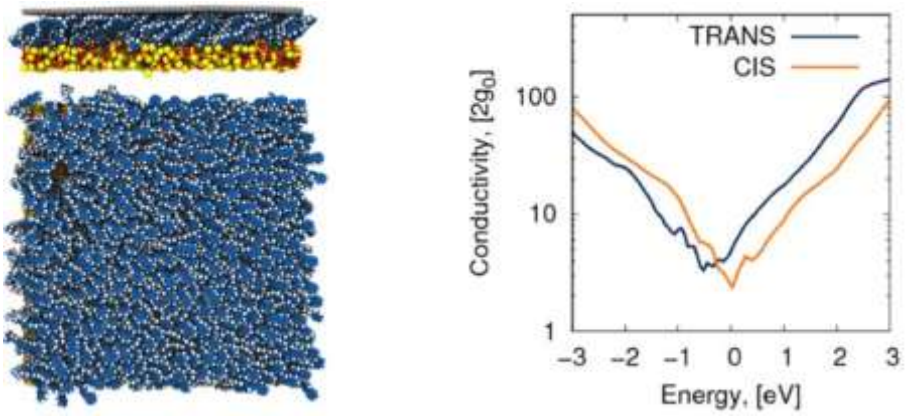

Figure 1: Side and top views of silica surface covered by self-assembled monolayer (SAM) of azobenzene molecules with graphene on top. The azobenzene surface density is 2.4 molecules per nm².