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Influence of structural fluctuations on lifetimes of adsorbate states at hybrid organic-semiconductor interfaces[1] M. MÜLLER, CIC nanoGUNE, San-Sebastián, D. SÁNCHEZ-PORTAL, CSIC, San-Sebastián, Spain, H. LIN, Univ. Milano-Bicocca, Italy, G. FRATESI, Univ. Milano, Italy, G.P. BRIVIO, Univ. Milano-Bicocca, Italy, A. SELLONI, Princeton Univ., USA — On the road towards a more realistic description of charge transfer processes at hybrid organic-semiconductor interfaces for photovoltaic applications we extend our first-principles scheme for the extraction of elastic linewidths to include the effects of structural fluctuations. Based on snapshots obtained from Car-Parinello molecular dynamics simulations at room temperature, we set up geometries in which dye molecules at interfaces are attached to a semi-infinite TiO_2 substrate. The elastic linewidths are computed using a Green's function method. This effectively introduces the coupling to a continuum of states in the substrate. In particular we investigate catechol and isonicotinic acid on rutile(110) and anatase(101) at the level of semi-local density functional theory. We perform multiple calculations of linewidths and peak-positions associated with the adsorbate's frontier orbitals for different geometric configurations to obtain a time-averaged analysis of such physical properties. We compare the results from the considered systems to understand the effects of dynamics onto interfacial charge transfer and systematically assess the dependence of the extracted elastic lifetimes on the relative alignment between adsorbate and substrate states.

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