Electronic screening of quasiparticle excitations by atomically thin substrates

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The weaker screening response within two-dimensional (2D) materials has manifested in novel physical phenomena, with strongly bound excitons being a well-known example. Here, we study the screening properties in reduced dimensions by employing first principles many-electron GW calculations, focusing on the electronic screening of point charge perturbations adjacent to a 2D material. We find that this is an excellent approximation for predicting the HOMO-LUMO gaps of benzene adsorbed on 2D materials, without expensive GW calculations for the full system. Interestingly, by comparing the screening response of ~15 2D and 3D substrates to point charge perturbations above the substrate, we find that both 2D and 3D substrates have a screening response that obeys the *same* approximately linear relation with their quasiparticle gaps. This is in contrast to the much weaker screening response of 2D materials to excitations *within* the material, and implies that 2D materials are effective atomically thin dielectrics. Our results can be attributed to the fact that most of the induced charge responding to the perturbing potential is located within ~2-3 Å of the surface atomic plane in both 2D and 3D substrates. We further develop a GW embedding model that enables the treatment of large supercells of organic monolayers interfaced with 2D materials, and apply the method to a prototypical system – an ordered herringbone structure of PTCDA molecules on a monolayer WSe_2 substrate. These results show that the non-locality of the screened Coulomb interaction and polarizability of the layer result in reduced screening in the PTCDA monolayer compared to that in a monolayer of smaller benzene molecules. Our work contributes to the ongoing effort in making GW calculations more tractable for large interface systems, and uncovers new insights into the unusual physics of screening in reduced dimensions.