Local dielectric permittivity profiles of sapphire/polypropylene interfaces

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Using first principles calculations, we have studied the optical and static dielectric permittivity profiles of the interface between α-Al_2O_3 and isotactic polypropylene. Our results indicate that (1) the dielectric permittivity approaches the corresponding bulk value just a few atomic layers away from the interface or surface; (2) the dielectric constant is enhanced at the surfaces of the isolated (0001/0110) α-Al_2O_3 slabs, while no enhancement is observed at the surfaces of a polyproylene slab; (3) the dielectric transition at the Al_2O_3/polypropylene interface occurs only within a few atomic layers and is mainly governed by chemical grading.