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First-principles study of multi-control doping using azobenzene adsorbed on graphene[1] JONATHAN TRINASTIC, HAI-PING CHENG, Quantum Theory Project, University of Florida — The high carrier mobility in graphene promises its utility in electronics applications, however more research is necessary to find optimal doping methods. Azobenzene (AB) is a widely used organic molecule for switchable optoelectronic devices that can be synthesized with a wide variety of ligands and deposited on graphene. Using first-principles calculations, we investigate the doping of graphene by physisorbed azobenzene molecules with various electron-donating and –accepting ligands. We confirm previous experimental results (Peimyoo et al 2011, *ACS Nano*,6(10),8878) that demonstrate greater p-doping of graphene for the *trans* compared to *cis* configuration when using a SO_3 electron-accepting ligand, and we find different levels of p-doping when using other ligands. We extend these findings by examining the doping effects of an applied electric field and applied strain to the graphene, which leads to changes in doping for both the *trans* and *cis* isomers. These findings demonstrate a new type of multi-switch device combining light, electric field, and strain to change carrier concentration in graphene.

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