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Electronic and Catalytic Properties of Iodine-Doped Graphene[1]
ROBERT A. HOYT, E. MARIELLE REMILLARD, EKIN D. CUBUK, CHAD D. VECITIS, EFTHIMIOS KAXIRAS, Harvard University — Polyiodide-doped graphene is an exciting recent material that exhibits significantly increased conductivity and oxygen reduction reaction (ORR) activity. Although polyiodide chains with a wide variety of lengths have been observed across a range of chemical systems, only I_3 and I_5 are observed as graphene dopants. In addition, while the mechanisms of ORR are understood for substitutionally-doped graphene, these polyiodides are reversible surface dopants so their role as active sites for ORR catalysis is unclear. To address these issues, we use density functional theory calculations to investigate the formation and desorption energies of isolated polyiodides on graphene, their electronic band structures, and degree of charge transfer. We also present results showing the stabilization of the OOH intermediate by I_3 on graphene, explaining the high ORR activity seen in polyiodide-doped graphene.

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