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**Electronic and structural properties of fluorinated graphene<sup>1</sup>**

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NRL, Washington, DC — Experiments have shown that the electronic structure of graphene can be tailored from that of a semimetal to that of a wide bandgap semiconductor through adsorption of fluorine. This makes fluorinated graphene  $C_xF$  ( $x \geq 1$ ) attractive for electronics applications. Here we present first-principle calculations that reveal the dependence of  $C_xF$  electronic structure on the degree of fluorination in the range  $1 \leq x \leq 8$ . We present a systematic analysis of bandgap opening and p-doping, as well as of adsorption energies, lattice constants, bulk modulus and surface corrugation for single-face and two-face functionalization. We rationalize these with a band-interpolation scheme in terms of localized orbitals that clarify the C-C, C-F and F-F bonding. We discuss the relevance of tunable Young modulus for nanomechanical resonators.

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