# Organic Metal-free Ferroelectric and Multiferroic Materials

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Ferroelectric materials, possessing spontaneous electric polarizations that are switchable under an external electric field, have a wide range of applications in electronics, micro-mechatronics, and electro-optics. Most of the current ferroelectric materials are based on inorganic elements. Using density functional theory we show that graphene based materials, functionalized with hydroxyl groups, constitute a class of multifunctional, lightweight, and nontoxic organic ferroelectric and multiferroic materials. For example, the polarizations of semi-hydroxylized graphane and graphone, as well as fully hydroxylized graphane, are much higher than any organic ferroelectric materials known to date. Further, hydroxylized graphene nanoribbons with proton vacancies at the end can have much larger dipole moments. They may also be applied as high-capacity cathode materials with a specific capacity that is six times larger than lead-acid batteries and five times that of lithium-ion batteries. Density functional theory has also been used to design of a variety of organic ferroelectric and multiferroic materials by functionalizing crystallized transition-metal molecular sandwich nanowires with chemical groups such as F, Cl, CN, $NO_2$, O, and OH. Such functionalized polar wires exhibit molecular reorientation in response to an electric field.