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Nanoscale Capacitors Composed of Graphene and Boron Nitride Layers: Size Effects at Small Separation V. ONGUN OZCELIK, SALIM CIRACI, Bilkent Univ — A nanoscale dielectric capacitor model consisting of two-dimensional, hexagonal h-BN layers placed between two commensurate and metallic graphene layers is investigated using self-consistent field density functional theory. The separation of equal amounts of electric charge of different sign in different graphene layers is achieved by applying electric field perpendicular to the layers. The stored charge, energy, and the electric potential difference generated between the metallic layers are calculated from the first-principles for the relaxed structures. Predicted high-capacitance values exhibit the characteristics of supercapacitors. The capacitive behavior of the present nanoscale model is compared with that of the classical Helmholtz model, which reveals crucial quantum size effects at small separations, which in turn recede as the separation between metallic planes increases.

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