Understanding and designing negative-compressibility materials from first principles

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Capacitors are ubiquitous in solid state devices like metal oxide semiconductors field effect transistors (MOSFET). The most important physical quantity to determine its performance is its capacitance. For energy efficiency, the MOSFET should operate at small gate voltages. In this regime, to increase the channel conductivity and performance, the capacitance of the capacitor between the gate and the channel should be made as large as possible. Assuming parallel plate capacitors, the classical capacitance is directly proportional to the lateral capacitor area and to its dielectric constant, and inversely proportional to its thickness. Recently, an enhancement of the capacitance of upto 40% with respect this classical limit has been reported in two-dimensional electron gases (2DEG) formed at the interface between two oxides, $SrTiO_3$ and $LaAlO_3$ [1]. A first theoretical analysis pointed to the quantum exchange-energy in the electron-electron interactions as the driving force to explain the anomalous behaviour [2]. The exchange-interaction would produce a lowering of the chemical potential of the electron system as the electronic density increases (the negative compressibility effect).

Here we test the validity of the approach, carrying out self-consistent calculations on a capacitor where the metallic plates are simulated by a jellium. We observe how the negative compressibility effect is obtained only in the limit of ultrathin electrodes. Moreover, the physical properties of the 2DEG at oxide interfaces might strongly deviate from the free-electron gas model of the jellium. Using second-principles approach to simulate the complete oxide capacitor, we will propose alternative scenarios that include the formation of polarons.

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