Abstract Submitted
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Quantum Stress: Density Functional Theory Formulation and Physical Manifestation[1] HAO HU, FENG LIU, Department of Materials Science and Engineering, University of Utah — The concept of "quantum stress (QS)" is introduced and formulated within density functional theory (DFT), to underlie extrinsic electronic effects on the stress state of solids and thin films in the absence of lattice strain. An explicit expression of QS (σ^Q) is derived in relation to the deformation potential of electronic states (Ξ) and the variation of electron density (Δn), $\sigma^Q = \Xi(\Delta n)$, as a quantum analog of classical Hook's law. Two distinct QS manifestations are demonstrated quantitatively by DFT calculations: (1) in the form of bulk stress induced by charge carriers; and (2) in the form of surface stress induced by quantum confinement. QS has broad implications in physical phenomena and technological applications that are based on coupling of electronic structure with lattice strain.

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