Abstract Submitted
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Surface and Quantum-Confinement Effects in Ultrathin MoSi2 films[1] LIANG-FENG HUANG, JAMES RONDINELLI, Northwestern University — Mo-Si-based alloys are promising structural materials for ultrahigh-temperature applications owing to their excellent mechanical strength at elevated temperature. Among the Mo-Si alloys, $MoSi_2$ exhibits outstanding oxidation resistance as a result of native SiO_2 scale formation. In this work, using density-functional theory calculations, we propose the alternative novel usage of $MoSi_2$ for nanoelectronics. The cleavage of $MoSi_2$ nanofilms from the layered bulk requires low energy because of the preserved chemical stoichiometry, indicating their facile synthesis in experiment. We explore the surface and quantum-confinement effects by investigating the thickness-dependent structure, stability, and electronic structure of $MoSi_2$ nanofilms, where high carrier concentrations have also been observed. The possible applications of $MoSi_2$ nanofilms as robust metallic substrates, electrodes, and in other nanodevices are discussed. In addition, we also discuss the effect of surface-induced metallicity on Raman spectra of $MoSi_2$, which are frequently used to characterize $MoSi_2$ samples.

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