

Abstract Submitted
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Effect of doping on lattice instabilities of 1H-TaS₂¹ OLIVER R. ALBERTINI, AMY Y. LIU, Georgetown University, MATTEO CALANDRA, CNRS and Université Pierre et Marie Curie — Recent ARPES measurements of single-layer 1H-TaS₂ grown on Au(111) suggest strong electron doping from the substrate.² In addition, STM/STS measurements on this system show the suppression of the charge-density-wave (CDW) and superconducting instabilities occurring in bulk 2H-TaS₂.² We present results from ab initio DFT calculations of free-standing single-layer 1H-TaS₂ to explore the effects of doping on the CDW. For the undoped monolayer, we find a lattice instability along the $\Gamma - M$ line, consistent with the bulk 3×3 CDW ordering vector. We then study the behaviour of the CDW instability as a function of doping from the substrate. We show that doping progressively removes the CDW instability, in agreement with the experimental findings. We explore the interplay between doping and strain, and we examine the electron-phonon coupling and the electronic susceptibility to understand the doping-induced changes in lattice instabilities.

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