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Low-Frequency Raman Modes of 2H-TaSe₂ in the Charge Density Wave Phase SUGATA CHOWDHURY, The Catholic University of America, J. SIMPSON, Towson University, T. L. EINSTEIN, University of Maryland, A. R. HIGHT WALKER, National Institute of Standards and Technology, THEORETICAL COLLABORATION — With changes in temperatures, tantalum diselenide (2H-TaSe₂), a layered, transition metal chalcogenides (TMD) exhibits unique superlattice structures. The metallic ground state changes to an incommensurate charge density wave (CDW) state at ≈ 122 K followed by a commensurate CDW state at ≈ 90 K, and eventually a superconducting state ≈ 0.14 K. These phase transitions are driven by strong electron-phonon coupling and favored by the particular form of the Fermi surface of these systems. Here we theoretically studied the structural origin of low-frequency Raman modes of bulk 2H-TaSe₂ in the CDW phases. Our calculations reveal that changes observed in the Raman modes are associated with the thermal expansion in the basal plane of 2H-TaSe₂. The Grüneisen parameters of these two Raman modes increase in the CDW phases. Changes in the lattice parameter “a” are large compared to “c” which induces strain along the a-axis. We compared our results with experimental data which show low-frequency Raman phonon modes are very sensitive to temperature and are not observed in the metallic room-temperature state. In addition, we found that cation displacement is more than anion in CDW phase. Our results may shed more light on exact nature of the CDW instability and optical properties in this system.

Sugata Chowdhury
The Catholic University of America
National Institute of Standards and Technology

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