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**Phonon Softening and Displacement Pattern in Commensurate Charge Density Wave in 2H-TaSe<sub>2</sub>** TOM BERLIJN, WEI-GUO YIN, WEI KU, Brookhaven National Laboratory — The formation of the commensurate charge density wave (CCDW) phase of 2H-TaSe<sub>2</sub> is investigated via a first-principles study of the phonon spectrum. Both the linear response and the frozen phonon approach reveal strong softening of the  $\Sigma_1$  branch at the CCDW wave vector ( $2\Gamma M/3$ ), as observed by inelastic neutron scattering[1]. Furthermore, to resolve the disagreement between currently proposed patterns by neutron scattering[1], electron diffraction[2] and TDPAC[3], the size and the pattern of the CCDW displacement are evaluated by an *abinitio* total energy calculation. The role of nesting and electron-phonon coupling in the microscopic origin of the instability will be addressed. [1] D.E. Moncton, J.D. Axe and F.J. DiSalvo, Phys. Rev. B **16**, 801 (1977), [2] D.M. Bird, S. McKernan and J.W. Steeds, J. Phys. C **18** 499 (1985), [3] T. Butz, S. Saibene and A. Lerf, J. Phys. C **19** 2675 (1986).

Prefer Oral Session  
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