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Phonons and excitons in $ZrSe_2$ – ZrS_2 alloys

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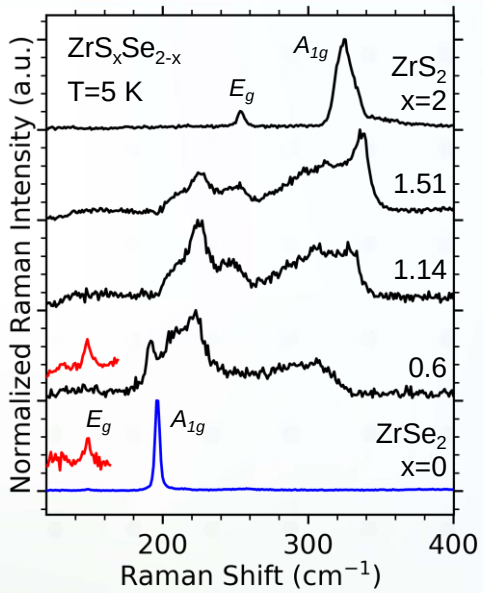
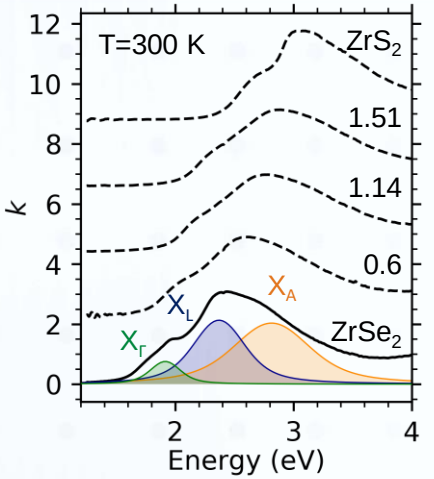
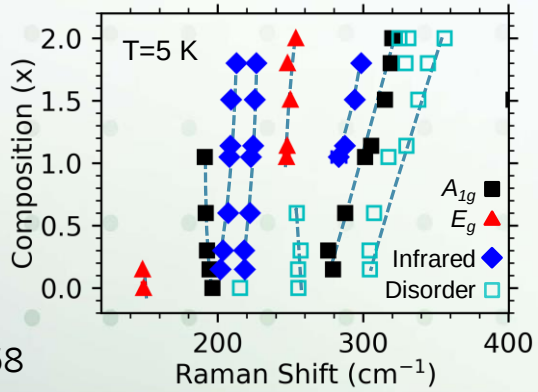
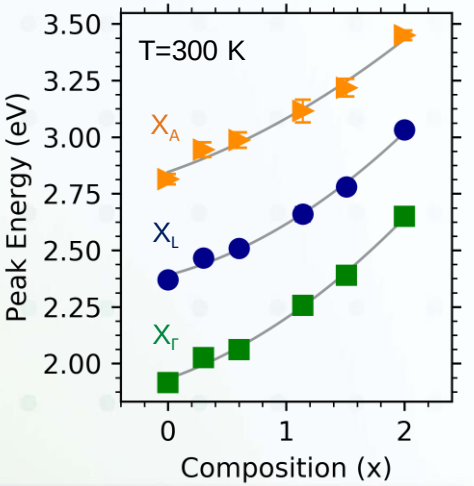
Sean M. Oliver, Joshua J. Fox, Arsalan Hashemi, Akshay Singh, Randal L. Cavalero, Sam Yee, David W. Snyder, Rafael Jaramillo, Hannu-Pekka Komsa, Patrick M. Vora

ZrS_2 has received increased attention due to its indirect band gap that matches with the visible spectrum and which is predicted to undergo an indirect-to-direct transition with strain. Alloying with $ZrSe_2$ to produce ZrS_xSe_{2-x} (x=0...2) would provide continuous control over key optical and electronic parameters for photonics. Here, we combine Raman spectroscopy, spectroscopic ellipsometry (SE), and density functional theory to conduct the first comprehensive exploration of phonons and excitons in this system. We find that long-range Coulomb interactions activate optically-silent infrared phonons that completely dominate Raman spectra in some alloys. SE measurements of excitons reveal strong light-matter interactions with low optical losses for near-infrared wavelengths. This study suggests ZrS_xSe_{2-x} alloys will find applications in atomically-thin, tunable photodetectors and photovoltaics.









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