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Stoichiometry driven impurity configurations in compound semiconductors[1]

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As is well known, crystal growth of defect-free compound semiconductors, in contrast to elemental, is inherently limited by non-stoichiometry. High resolution infrared spectroscopy of localized vibrational modes can display unique signatures which reveal the structure of stoichiometry related defect-impurity complexes. The talk will focus on II-VI semiconductors in which group II cations are replaced with a group IIA or a 3d-transition metal ion as an impurity, on the one hand, and a group VI anion replaced with a group VIA impurity, on the other. Incorporation of O replacing Te with a full complement of nearest neighbor Cd's, i.e. O_{Te}, as well as O_{Te} in association with a Cd vacancy (V_{Cd}) in the zincblende CdTe result in defect centers with unique i.r. signatures. The occurrence of O_{Te} with T_d symmetry and ($O_{Te} - V_{Cd}$) with C_{3v} symmetry can be controlled by favoring or suppressing Cd vacancies. In CdSe, with its wurtzite structure, oxygen incorporation occurs in two ways: in one, it is an "anti-site" defect, O_{Cd}, as revealed in its host isotope related fine structure; in the other, oxygen enters in association with Cd vacancies as ($O_{Se} - V_{Cd}$). The talk will discuss the number of i.r. signatures specific to each center; their polarization characteristics (in CdSe); the striking temperature behavior of the i.r. signatures of ($O_{Te} - V_{Cd}$) and ($O_{Se} - V_{Cd}$); and the occurrence of overtones/combinations of the LVMs in CdTe. These investigations provide a wealth of microscopic insights into orientational degeneracy, host isotope effects and acquisition of the temperature averaged higher symmetries by the switchings of the dangling bond of V_{Cd}.

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