

物理工学談話会 5月22日(木) 午後13:30~

会場：総合研究棟W202 世話人：レービガー ハンネス

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Density functional study of phonon-induced photocarrier capture in defective MoSe₂

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In recent years, optical electronic excitations and photocarrier dynamics in transition metal dichalcogenides (TMDCs) have been actively investigated in view of understanding photophysics in atomically thin materials and their optical device applications. According to recent studies on pristine TMDCs, acoustic phonons are involved in exciton generation and electron cooling processes [1,2]. In practical situations, TMDC samples usually contain a certain amount of defects and adsorbates, which act as ultrafast photocarrier trapping centers [3,4]. Meanwhile, although the exciton-phonon interaction in pristine TMDC is relatively well studied, defect-related photocarrier trappings remain vague.

Here, we present our theoretical study of defect-induced photocarrier capture in MoSe₂ by means of delta-self-consistent-field (Δ SCF) density functional theory calculations [5,6]. Starting from the ground-state MoSe₂ with various defects, we explicitly minimize the geometry of its excited states at defects, thus explicitly treating the nonradiative decay through multi-phonon emission processes. Comparing our computational results with pump-probe measurement data, we conclude that the exciton trapping at a Se vacancy adsorbed by an oxygen molecule is a dominant photocarrier capture mechanism.

- [1] S. Shree, *et al.* Phys. Rev. B **98**, 035302 (2018).
- [2] C.M. Chow, *et al.* npj 2D Mater. Appl. **1**, 33 (2017).
- [3] K. Chen, *et al.* Adva. Mater. **28**, 5293 (2016).
- [4] H. Chuan, *et al.* ACS Appl. Mater. Interfaces **10**, 1125-1131 (2018)
- [5] A. Gail, *et al.* Phys. Rev. B **80**, 241204 (2009).
- [6] A. Alkauskas, *et al.* J. Appl. Phys. **119**, 18 (2016).