DEFECTS IN TWO-DIMENSIONAL INORGANIC MATERIALS

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Following isolation of a single sheet of graphene, many other 2D systems such as hexagonal BN sheets and transition metal dichalcogenides (TMD) were manufactured. Among them, TMD sheets have received particular attention, as these materials exhibit intriguing electronic and optical properties. Moreover, the properties can further be tuned by introduction of defects and impurities. In my talk, I will present the results [1] of our first-principles theoretical studies of defects (native and irradiation-induced) in graphene and inorganic 2D systems obtained in collaboration with several experimental groups. I will further discuss defect- and impurity-mediated engineering of the electronic structure of 2D materials.

Keywords: 2D materials, defects, transmission electron microscopy, first-principles calculations

References

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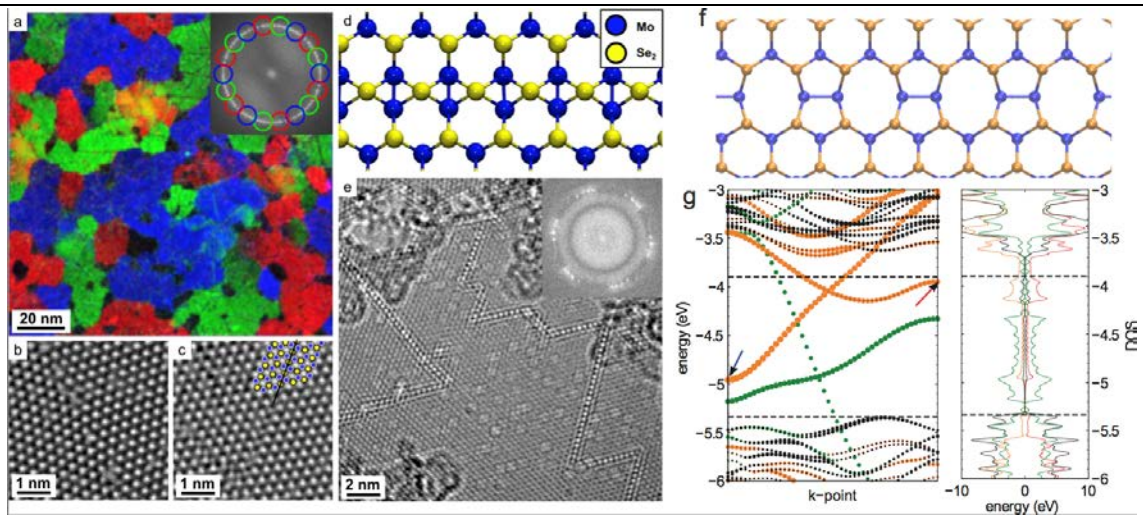

Line defects in inorganic 2D TMDs. (a) The grain structure, with the color coding corresponding to different grain orientations in $MoSe_2$ [from Ref.4]. (b) A close-up view of a tilt grain boundary. c: A close-view of a mirror-twin-boundary within a grain. (d) The theoretical structure, as calculated using DFT. (e) A larger field of view image. Single vacancies are also visible. (f) Atomic structure of another type of mirror twin boundary structure (composed from 5-8 membered rings) observed in WSe_2 [from Ref.1]. (g) Band structure and density of states of a mirror twin boundary in TMD.