THEOROTICAL ELECTRON SCATTERING STUDIES WITH ATOMIC MOLYBDENUM AND MOS_2

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Electron impact ionization (EI) is one of the primary processes in plasmas and its cross section is of overriding importance to model fusion plasmas and astrophysical plasmas. In fusion plasmas it is well known that many kinds of impurity ions exist due to the sputtering of the wall materials. The understanding of the atomic processes of the elements with industrial importance such as Mo is also essential to control the impurity ions in plasmas [1] .
The calculations on Molybdenum are also of interest in divertor studies in several experimental facilities, where a spectroscopic determination of impurity influx from the molybdenum surface is needed. One of the outstanding challenges in applied plasma physics is the development of non-mercury gas discharges for lighting. The discovery of grapheme nearly a decade ago has stimulated intensive research efforts in atomically thin, two-dimensional (2D) crystals, such as transition-metal dichalcogenide (TMD) semiconductors and boron-nitride BN.Compared to graphene, the presence of a bandgap in TMDs is more desirable for device applications. Recent experimental and theoretical work shows that these layered TMDs undergo a transition from indirect to direct bandgap when their thickness is reduced from bulk to monolayer, leading to a pronounced photoluminescence (PL). Among this family, Molybdenum Disulfide is one of the most stable layered TMDs [2].
In this backdrop, the present paper reports comprehensive theoretical investigations on electron scattering with atomic molybdenum and Molybdenum Disulfide. The spherical complex (optical) potential formalism (SCOP) is applied here, which provides total elastic cross section and its inelastic counterpart which includes ionization cross section. A method to extract ionization cross sections from calculated inelastic cross-sections is developed by introducing a ratio function as in [3]. The calculated cross sections are examined as functions of incident electron energy along with available comparisons. Detailed analysis of the results will be presented in the workshop.

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