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Symmetry analysis of phonons in two-dimensional Transition Metal Dichalcogenides

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The interest in two-dimensional (2D) layered materials increased after the successful isolation of monolayer graphene reported in 2004 [1]. The monolayer of hexagonally-linked carbon atoms made it possible to study a brand-new set of electric, and optical phenomena, but the lack of a band gap imposes some difficulties to graphene's application in electronics, despite its high carrier mobility. Other classes of 2Dmaterials are now also being intensively studied for many different applications motivated mainly by the need of a band gap. The family of transition metal dichalcogenides (TMDCs), such as MoS2 and WSe2, offer a wide range of compounds and combinations with potential use in the emerging field of 2D heterostructures. The TMDCs are layered materials of the form MX2, where M stands for groups IV–X of transition metals and X stands for the chalcogen atoms S, Se, or Te. Some monolayer semiconducting TMDCs show a direct band gap in the visible range, which does not exist in their bulk counterparts. These band gaps open the possibility for flexible and transparent sensor applications, and tunable optoelectronic properties obtained by a suitable choice of component layers in atomically thick heterostructures [2].
The exfoliation of these TMDCs generates the breaking of translational symmetry in the direction perpendicular to the layers planes. Previous works have shown the appearance of new modes in few-layer TMDCs Raman spectra related to symmetry variations, as well as non-linear optical response that is dependent of the layer number. Here we apply the group theory formalism to address symmetry aspects that are layer number dependent, for three different TMDCs stacking orders (2Ha, 2Hc and 1T polytypes), and with different transition metal atom coordination [trigonal prismatic (H) and octahedral (T)]. We go beyond the Brillouin Zone center phonons, showing the irreducible representations for the lattice vibration for other high-symmetry lines and points in the reciprocal space, and its respective group of the wave vector. The number of Raman and infrared active modes is given for the different polytypes, and bulk related data are compared. The results can be applied to a family of more than 30 layered compounds that exhibit different electrical, mechanical and optical properties, and are suitable for further examination of symmetry-breaking induced effects. [1] K. S. Novoselov, et al. Science, 306(5696):666–669, 2004. [2] H. Fang et al. P. Natl. Acad. Sci. USA, 111(17):6198–6202, 2014.

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