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**The electronic and transport properties of monolayer transition metal dichalcogenides: a complex band structure analysis**[1] DOMINIK SZCZESNIAK, Qatar Energy and Environment Research Institute, Hamad bin Khalifa University, Qatar Foundation — Recently, monolayer transition metal dichalcogenides have attracted much attention due to their potential use in both nano- and opto-electronics. In such applications, the electronic and transport properties of group-VIB transition metal dichalcogenides ($MX_2$, where $M$=Mo, W; $X$=S, Se, Te) are particularly important. Herein, new insight into these properties is presented by studying the complex band structures (CBS's) of $MX_2$ monolayers while accounting for spin-orbit coupling effects. By using the symmetry-based tight-binding model a nonlinear generalized eigenvalue problem for CBS's is obtained. An efficient method for solving such class of problems is presented and gives a complete set of physically relevant solutions. Next, these solutions are characterized and classified into propagating and evanescent states, where the latter states present not only monotonic but also oscillatory decay character. It is observed that some of the oscillatory evanescent states create characteristic complex loops at the direct band gaps, which describe the tunneling currents in the $MX_2$ materials. The importance of CBS's and tunneling currents is demonstrated by the analysis of the quantum transport across $MX_2$ monolayers within phase field matching theory.

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