

# First principle investigation on thermoelectric properties of transition metal dichalcogenides: Beyond rigid band model

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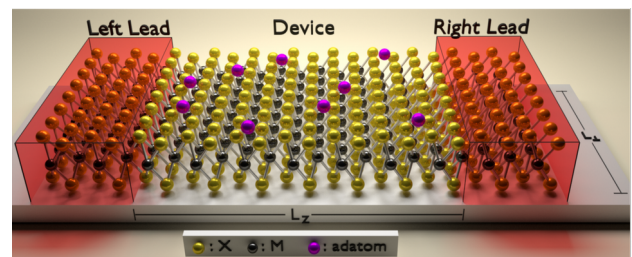
Two-dimensional direct band-gap transition-metal dichalcogenides (TMDC) with chemical composition  $\text{MX}_2$  ( $M=\text{Mo}$  or  $\text{W}$  and  $X=\text{S}$  or  $\text{Se}$ ) have led to a growing interest in the last decade. For instance, in the field of nanoelectronic, significant accomplishments have been done in the development of  $\text{MoS}_2$  based transistors.

We have investigated the thermoelectric properties (electrical conductivity, Seebeck coefficient and power factor) of single layer TMDC on the basis of *ab initio* quantum transport using Landauer Büttiker formalism (see **Figure 1**). The often used rigid band model is compared to realistic doping, namely substitution and adsorption, it is found that several important physical insights governing the transport are missing in this approximation. The rigid band model appears to clearly overestimate the thermoelectric efficiency, hampering its relevance for thermoelectric studies. Substitution doping by chloride or phosphorus leads to poor power factor due to drastic changes of the pristine band structure. In contrast, adsorption doping by alkalis (Li, Na, K and Rb) favors larger power factor (see **Figure 2**).

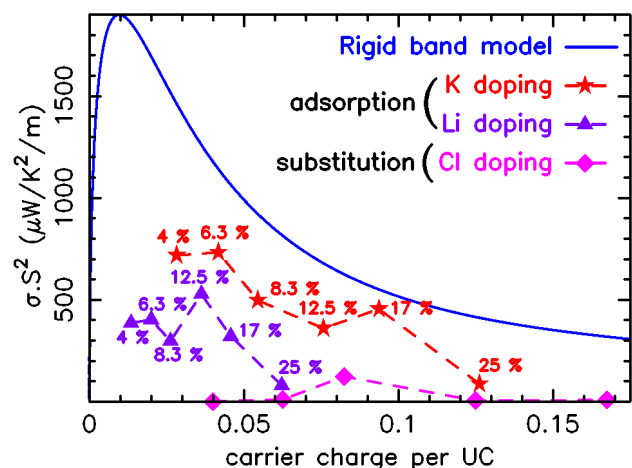
Thanks to the Landauer formalism, a realistic treatment of the disorder induced by the dopants is also investigated and reveals that Cl doping leads to very short localization length of 3.5 nm whilst K comes with micrometer length scale. The Anderson localization phenomenon in thermoelectric properties of single layer transition metal

dichalcogenides definitely comes out as a main issue.

## Figures



**Figure 1.** Schematic representation of the system within the Landauer formalism.



**Figure 2.** Power factor for  $\text{MoS}_2$  with 3 different dopants: K, Li and Cl, as well as the rigid band calculation.