Journal Name

ARTICLE TYPE

Cite this: DOI: 10.1039/xxxxxxxxxx

Electro-vibrational Coupling Effects on "Intrinsic Friction" in Transition Metal Dichalcogenides - Electronic Supplementary Information

Antonio Cammarata,*[a] and Tomas Polcar[b]

Received Date
Accepted Date

DOI: 10.1039/xxxxxxxxxx

www.rsc.org/journalname

1 Cophonicity Metric

Let's consider the phonon density of states (pDOS) $g(\omega)$. We define the center mass cm^A of the atom-projected pDOS $g^A(\omega)$ of an atom A as

$$cm^A \equiv \frac{\int_{\omega_0}^{\omega_1} \omega g^A(\omega)\, d\omega}{\int_{\omega_0}^{\omega_1} g^A(\omega)\, d\omega} \tag{1}$$

where we call $g^A(\omega)$ the contribution of the atom A to $g(\omega)$ and $\omega_1 > \omega_0$; $g(\omega)$ is the total pDOS of the system

$$g(\omega) = \sum_A g^A(\omega) \tag{2}$$

and is calculated by summing over all atoms A of the unit cell. The integration interval $[\omega_0, \omega_1]$ in Equation 1 is chosen so as to consider all the phonon states relevant for the selected band. The integral at the denominator of the definition of cm^A is the contribution of the atom A to the states in the frequency range $[\omega_0, \omega_1]$; we call such quantity *phonicity of the A atom* in the $[\omega_0, \omega_1]$ frequency range. The phonicity of an atom then represents the amount of phonon states that such atom contributes to form; in this respect, we can think to it as the phonon counterpart of the atomic valence, that is the number of electrons that an atom provides to form the electronic states of the system, such number counted as the integral of the atom-projected electronic density of states.

Let's now consider a generic A-B atomic pair. The relative position C_{ph}(A-B) of the center mass of $g^A(\omega)$ with respect to the center mass of $g^B(\omega)$ is given as

$$C_{ph}(\text{A-B}) = cm^A - cm^B; \tag{3}$$

C_{ph} is thus specified in the same units of the frequency ω. In this formalism, a positive (negative) sign of C_{ph}(A-B) indicates that the A (B) atom contributes more to the high frequency modes of the specified range. The smaller is the absolute value of C_{ph}(A-B), the higher is the mixing of the A and B contributions to the frequency band; the two atoms then have the same weight in the formation of the modes specific of the considered energy range. We define the quantity C_{ph}(A-B) as the *cophonicity of the A-B atomic pair*,[1] in analogy with the A–B bond covalency definition formulated for crystalline compounds.[2]

[a] *Department of Control Engineering, Czech Technical University in Prague, Technicka 2, 16627 Prague 6, Czech Republic. Fax: +420 224 91 8646; Tel: +420 224 35 7598; E-mail: cammaant@fel.cvut.cz*

[b] *Engineering Materials & nCATS, FEE, University of Southampton, SO17 1BJ Southampton, United Kingdom.*

References

1 Cammarata, A.; Polcar, T. *Inorganic Chemistry* **2015**, *54*, 5739–5744.

2 Cammarata, A.; Rondinelli, J. M. *J. Chem. Phys.* **2014**, *141*, 114704.