Erratum: Two-dimensional Fröhlich interaction in transition-metal dichalcogenide monolayers: Theoretical modeling and first-principles calculations [Phys. Rev. B 94, 085415 (2016)]

Thibault Sohier, Matteo Calandra, and Francesco Mauri
(Received 16 October 2017; published 27 October 2017)

DOI: 10.1103/PhysRevB.96.159904

After the publication of the paper, a bug in the QUANTUM ESPRESSO (QE) distribution concerning the calculation of Born effective charges in the presence of nonlinear core corrections was corrected. Since all the pseudopotentials used included nonlinear core corrections, below we update the tables containing data affected by the bug. In practice, this leads to changes of a few percent in the Born effective charges and in the bare Fröhlich interaction (computed via the Born effective charges). Importantly, the latter parameter is now much closer to the corresponding value fitted on direct electron-phonon calculations. This bug thus explains the previously observed mismatch discussed in the second paragraph of Sec. V of the original paper. The other results, and in particular the figures, were computed via direct phonon calculations and were not affected by the bug.

TABLE II. Dielectric constants and effective charges of bulk and monolayer MoS_2 as obtained in density functional theory. In the case of the monolayer, we report the dielectric constant in the case of an isotropic model. The full range of possible values for the in-plane and out-of-plane dielectric constants is given in Fig. 5.

Bulk		Monolayer	
Symbol	Value	Symbol	Value
ϵ^b_p	15.37	$\epsilon^m_p = \epsilon^m_{\rm iso}$	15.5
ϵ^b_z	6.57	$\epsilon^m_z = \epsilon^m_{\rm iso}$	15.5
$Z^b_{{\rm Mo},p}$	−0.97796	$Z^m_{{\rm Mo},p}$	−1.00475
$Z^b_{{\rm Mo},z}$	−0.60102	$Z^m_{{\rm Mo},z}$	−0.11665
$Z^b_{{\rm S},p}$	0.48438	$Z^m_{{\rm S},p}$	0.50249
$Z^b_{{\rm S},z}$	0.30014	$Z^m_{{\rm S},z}$	0.05789

TABLE III. Effective charges of monolayer transition-metal dichalcogenides (TMDs) as computed in QE via the response to an external electric field. $M \equiv$ Mo,W. $X \equiv$ S,Se,Te.

Monolayer	$Z^m_{M,p}$	$Z^m_{M,z}$	$Z^m_{X,p}$	$Z^m_{X,z}$
MoS_2	−1.00	−0.12	0.50	0.06
$MoSe_2$	−1.78	−0.10	0.89	0.05
$MoTe_2$	−3.14	−0.14	1.57	0.07
WS_2	−0.48	−0.04	0.24	0.02
WSe_2	−1.16	−0.07	0.58	0.03

TABLE IV. Comparison of relevant quantities involved in the Fröhlich interaction for the monolayer TMDs MoS_2, $MoSe_2$, $MoTe_2$, WS_2, and WSe_2. a_0 is the lattice parameter. We report here the dielectric constants associated with the simplest isotropic model, that is, $\epsilon^m_{\rm iso} = \epsilon^m_p = \epsilon^m_z$ and $t = t_{\rm iso}$. Note that we use the fact that $r_{\rm eff} \approx \epsilon^m_{\rm iso} t_{\rm iso}/2$. For the bare Fröhlich interaction $C_{\mathcal{Z}}$, we report both the fitted value (from the fit) used in the plots to reproduce the density functional perturbation theory data and the value found by computing effective charges and phonons eigenvectors (*ab initio*).

Monolayer	a_0 (Å)	$t_{\rm iso}$ (Å)	$\epsilon^m_{\rm iso}$	$r_{\rm eff}$ (Å)	$C_{\mathcal{Z}}$ (eV) (from the fit)	$C_{\mathcal{Z}}$ (eV) (*ab initio*)	$\omega_{\rm LO}$ (cm^{-1})	$\omega_{\rm A_1}$ (cm^{-1})
MoS_2	3.18	6.00	15.5	46.5	0.355	0.355	373.7	396.9
$MoSe_2$	3.32	5.94	17.9	53.2	0.521	0.536	277.5	235.4
$MoTe_2$	3.56	6.65	20.9	69.5	0.819	0.849	223.6	162.9
WS_2	3.18	5.52	15.2	42.0	0.165	0.159	345.9	407.4
WSe_2	3.31	5.97	16.3	48.7	0.323	0.317	239.4	242.1

