PRAGMATIC BAND GAP CALCULATIONS AS A 'SIEVE' FOR EXPERIMENTAL TABULATIONS

D. M. Tomecka[1,*], S. Cottenier[1,2], V. Van Speybroeck[1], and M. Waroquier[1]

[1]Center for Molecular Modeling, Ghent University, Technologiepark 903, BE-9052 Zwijnaarde, Belgium
[2]Department of Materials Science and Engineering, Ghent University, Technologiepark 903, BE-9052 Zwijnaarde, Belgium

In this contribution we present calculated band gaps for a set of ca. 200 semiconductors for which experimental band gaps are available in standard tabulations [1]. Calculations were performed with the LAPW method implemented in the WIEN2k code [2], using the PBE and modified Becke-Johnson (mBJ) functionals. Correlations between the two sets of calculations and experiment will be presented and discussed, as well as correlations between the two sets of calculations themselves. It will be shown to which extent such an approach can be used to identify 'suspicious' entries in tabulated experimental data.

References

[1] CRC Handbook of Chemistry and Physics, CRC Press, 89th Edition, David R. Lide, Taylor & Francis Group, Boca Raton, FL, USA, 2008. ISBN13: 978-1-4200-6679-1.

[2] P. Blaha et al., WIEN2K, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties (Karlheinz Schwarz, Techn. Universitaet Wien, Austria), 1999. ISBN 3-9501031-1-2.

*)Corresponding author; e-mail: daria.tomecka@ugent.be