Contribution ID: **51** Type: **Talk**

The all-electron APW code WIEN2k: Applications to phonon related properties

Thursday, 5 December 2019 11:30 (35 minutes)

I will give a review on augmented plane wave (APW) methods for the calculation of the electronic structure in solids starting with the original concept developed by J. Slater [1] long time ago up to the APW+lo method introduced by Sjöstedt {\it et al.} [2]. This latter method combines the superior convergence behaviour of the original APW method with the convenience of LAPW [3]. I will then give an overview of the implementation of APW+lo into the WIEN2k code [4] and summarize the available features and discuss in particular the possibilities connected with calculations of phonons.
Selected results will be discussed in more detail. This will include phase transitions in $RbCaF_3$ [5] and $PbTiO_3$ [6] as well as a finite temperature (phonon) related explanation of a double peak occurring in the B-K XANES spectra of h-BN [7].

Refs
[1] J. Slater, Phys. Rev. {\bf 51}, 151 (1937).
[2] E. Sjöstedt, L. Nordström and D. Singh, Solid State Commun. {\bf 114}, 15 (2000).
[3] G. K. H. Madsen, P. Blaha, K. Schwarz, E. Sjöstedt and L. Nordström, Phys. Rev. B {\bf 64}, 195134 (2001).
[4] http://www.wien2k.at
[5] S. Ehsan, A. Tröster, F. Tran and P. Blaha, Phys Rev. Mat. {\bf 2}, 093610 (2018).
[6] A. Tröster, S. Ehsan, K. Belbase, P. Blaha, J. Kreisel and W. Schranz, Phys. Rev. B {\bf 95}, 064111 (2017).
[7] F. Karsai, M. Humer, E. Flage-Larsen, P. Blaha and G. Kresse, Phys. Rev. B {\bf 98}, 235205 (2018).

Primary author: BLAHA, Peter (Institute of Materials Chemistry, Vienna University of Technology, Austria)

Presenter: BLAHA, Peter (Institute of Materials Chemistry, Vienna University of Technology, Austria)

Track Classification: Methods