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Application of nuclear inelastic scattering spectroscopy to the frequency scale calibration of ab initio calculated phonon density of states of quasi-one-dimensional ternary iron chalcogenide rbfese2

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Abstract

© 2020 by the authors. Licensee MDPI, Basel, Switzerland. This study aims to examine the applicability of nuclear inelastic scattering (NIS) and conventional Mössbauer spectroscopy for calibration of the frequency scale of ab initio calculated phonon density of states (PDOS) of iron ternary chalcogenides. NIS measurements are carried out on the quasi-one-dimensional ternary chalcogenide RbFeSe2 to obtain the partial PDOS of the iron atoms in the compound. We compare the experimental PDOS with our previous results on vibrational properties of RbFeSe2 obtained with density functional theory (DFT) ab initio calculations, conventional Mössbauer, and infra-red spectroscopies. The experimental PDOS measured by NIS is collated with the ab initio calculated one. The frequency correction factor for the ab initio results is determined as 1.077, in good agreement with value of 1.08 obtained previously from the temperature dependence of the Lamb–Mössbauer factor of the iron atoms in RbFeSe2 . We conclude that nuclear inelastic scattering and temperature dependence of the Lamb–Mössbauer factor in conventional Mössbauer spectroscopy can be equally applied for evaluation of the frequency correction factor for ab initio calculated phonon density of iron of ternary chalcogenides.

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Keywords

Ab initio DFT theory, DFT phonon frequency correction factor, Nuclear inelastic scattering, Phonon density of states

References

[1] Fu, H.H.; Yao, K.L.; Liu, Z.L. Specific heat study on a spin-one-half frustrated diamond chain. Phys. Lett. A 2006, 358, 443–447. [CrossRef]

[2] Lysogorskiy, Y.V.; Eremina, R.M.; Gavrilova, T.P.; Nedopekin, O.V.; Tayurskii, D.A. Vibrational and magnetic properties of crystalline CuTe O . JETP Lett. 2015, 100, 652–656. [CrossRef]

[3] Kiiamov, A.G.; Lysogorskiy, Y.V.; Vagizov, F.G.; Tagirov, L.R.; Tayurskii, D.A.; Seidov, Z.; Krug von Nidda, H.A.; Tsurkan, V.; Croitori, D.; Günther, A.; et al. Vibrational properties and magnetic specific heat of the covalent chain antiferromagnet RbFeSe . Phys. Rev. B 2018, 98, 214411. [CrossRef]

[4] Kittel, C. Introduction to Solid State Physics, 7th ed.; John Wiley & Sons, Inc.: Hoboken, NJ, USA, 1996; Chapter 5.

[5] Seidov, Z.; Krug von Nidda, H.A.; Tsurkan, V.; Filippova, I.G.; Günther, A.; Gavrilova, T.P.; Vagizov, F.G.; Kiiamov, A.G.; Tagirov, L.R.; Loidl, A. Magnetic properties of the covalent chain antiferromagnet RbFeSe . Phys. Rev. B 2016, 94, 134414. [CrossRef]

[6] Parlinski, K.; Li, Z.; Kawazoe, Y. First-Principles Determination of the Soft Mode in Cubic ZrO . Phys. Rev. Lett. 1997, 78, 4063. [CrossRef]

[7] Braïda, B.; Hiberty, P.C.; Savin, A.A. Systematic Failing of Current Density Functionals: Overestimation of Two-Center Three-Electron Bonding Energies. J. Phys. Chem. A 1998, 102, 7872–7877. [CrossRef]

[8] Grinberg, I.; Ramer, N.J.; Rappe, A.M. Quantitative criteria for transferable pseudopotentials in density functional theory. Phys. Rev. B 2001, 63, 201102. [CrossRef]

[9] Gütlich, P.; Bill, E.; Trautwein, A.X. Mössbauer Spectroscopy and Transition Metal Chemistry. Fundamentals and Applications, 1st ed.; Springer: Berlin, Germany, 2011; pp. 7–24.

[10] Dorner, B. Coherent Inelastic Neutron Scattering in Lattice Dynamics; Springer Tracts in Modern Physics v.93; Springer: Berlin/Heidelberg, Germany; New York, NY, USA, 1982; p. 102.

[11] Chumakov, A.; Rüffer, R. Nuclear inelastic scattering. Hyperfine Interact. 1998, 113, 59–79. [CrossRef]

[12] Rüffer, R.; Chumakov, A.I. Nuclear inelastic scattering. Hyperfine Interact. 2000, 128, 255–272. [CrossRef]

[13] Wille, H.C.; Franz, H.; Röhlsberger, R.; Caliebe, W.A.; Dill, F.U. Nuclear resonant scattering at PETRA III: Brillant opportunities for nano-and extreme condition science. J. Phys. Conf. Ser. 2009, 217, 012008. [CrossRef]

[14] Kohn, V.G.; Chumakov, A.I. DOS: Evaluation of phonon density of states from nuclear resonant inelastic absorption. Hyperfine Interact. 2000, 125, 205–221. [CrossRef]

[15] Kresse, G.; Hafner, J. Ab initio molecular dynamics for liquid metals. Phys. Rev. B 1993, 47, 558–561. [CrossRef]

[16] Kresse, G.; Hafner, J. Ab initio molecular-dynamics simulation of the liquid-metal–amorphous-semiconductor transition in germanium. Phys. Rev. B 1994, 49, 14251. [CrossRef]

[17] Kresse, G.; Furthmuller, J. Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set. Comput. Mater. Sci. 1996, 6, 15–50. [CrossRef]

[18] Kresse, G.; Furthmuller, J. Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set. Phys. Rev. B 1996, 54, 11169–11186. [CrossRef] [PubMed]

[19] Perdew, J.P.; Burke, K.; Ernzerhof, M. Generalized Gradient Approximation Made Simple. Phys. Rev. Lett. 1996, 77, 3865–3868. [CrossRef] [PubMed]

[20] Blöchl, P.E. Projector augmented-wave method. Phys. Rev. B 1994, 50, 17953–17979. [CrossRef] [PubMed]

[21] Monkhorst, H.J.; Pack, J.D. Special points for Brillouin-zone integrations. Phys. Rev. B 1976, 13, 5188–5192. [CrossRef]

[22] Bronger, W.; Kyas, A.; Müller, P. The antiferromagnetic structures of KFeS, RbFeS, KFeSe, and RbFeSe and the correlation between magnetic moments and crystal field calculations. J. Solid State Chem. 1987, 70, 262–270. [CrossRef]

[23] Bronger, W.; Müller, P. The magnetochemical characterisation of the bonding features in ternary chalcogenides of manganese, iron aad cobalt with low dimensional structural units. J. Alloys Compd. 1997, 246, 27–36. [CrossRef]