Seminar on Condensed Matter Theory

Group of Theoretical Physics at the Department of Condensend Matter Physics of Charles University has a pleasure to invite you to attend the seminar

on 5 March 2021 at 13:00
as an online webinar

Contact K. Carva (carva@karlov.mff.cuni.cz) for the online access information.

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Thermal expansion and thermal conductivity of novel nuclear fuels

Actinides and especially their carbides as prospective nuclear fuel materials for the generationIV reactors were investigated using the density functional theory. We demonstrate that their electronic, magnetic, elastic, and thermal properties can be at present well described if the spin-orbit interaction and partial delocalization 5f electrons is properly included in the computational approaches. One can well reproduce not only basic electronic structure but also elastic constants, phonon dispersions, and their density of states, provided by XPS, UPS, BIS, and inelastic neutron scattering data [1-5]. Often, the localization of the 5f electrons could be captured using a moderate value of the on-site Coulomb interaction parameter. The case studies include a realistic description of the ground-state properties of elemental metals as Th, U and their monocarbides ThC and UC. In this study, published in Ref. 2 and 5, the realistic description of the electronic structure and lattice dynamics (phonons) explains why there is much higher thermal expansion and heat capacity in pure actinides (as Th) comparing with respective actinide monocarbides. The modeling also gives an insight up to which temperature the heat transport depends on lattice vibrations and where the electron transport starts to dominate. We identified the vibration mode that carries the most heat and what is the most limiting parameter. Also, we found that the phonon heat transfer is essentially the same for Th and ThC, despite the latter having large dispersive optical modes. These modes carry not more than 6% of phonon thermal conductivity. This is in huge contrast to actinide oxides, where the major role is played by optical phonon branches, their contributions up to 30% [3]. In Ref. 5 we additionally investigated defected UC, a more realistic situation often encountered, due to the self-irradiatons. The effects of vacancies at carbon site and oxygen impurities on the thermal expansion, heat capacity, and the phonon density of states (DOS) were compared to the experimental data in the large temperature scan showing very excellent agreement up to 2000K and explained some additional features of phonon DOS not presented before.

[1] U. D. Wdowik, P. Piekarz, D. Legut, and G. Jaglo, Phys. Rev. B 94, 054303 (2016).
[2] L. Kyvala and D. Legut (accepted PRB January 2020).

For more information follow: theory.kfkl.cz/seminars.php
If you wish to receive regular updates on fothcoming seminars, contact K. Carva (carva@karlov.mff.cuni.cz).

[3] P. Maldonado, L. Paolasini, P. M. Oppeneer, T. R. Forrest, A. Prodi, N. Magnani, A. Bosak,R. Caciuffo, Phys. Rev. B 93, 144301 (2016).
[4] Y. Yun, D. Legut and P. M. Oppeneer, J. Nucl. Mat. 426, 109 (2012).
[5] U. D. Wdowik, V. Buturlim, L. Havela, and D. Legut, J. Nucl. Mat. 545, 152547 (2021).