High-pressure study of binary thorium compounds from first principles theory and comparisons with experiment - DTU Orbit (11/12/2018)

High-pressure study of binary thorium compounds from first principles theory and comparisons with experiment
The high-pressure structural behaviour of a series of binary thorium compounds ThX (X = C, N, P, As, Sb, Bi, S, Se, Te) is studied using the all-electron full potential linear muffin-tin orbital (FP-LMTO) method within the generalized gradient approximation (GGA) for the exchange and correlation potential. The calculated equilibrium lattice parameters and bulk moduli, as well as the equations of state agree well with experimental results. New experiments are reported for ThBi and ThN. Calculations are performed for the ThX compounds in the NaCl-and CsCl-type crystal structures, and structural phase transitions from NaCl to CsCl are found in ThP, ThAs, ThSb and ThSe at pressures of 26.1, 22.1, 8.1 and 23.2 GPa, respectively, in excellent agreement with experimental results. ThC, ThN and ThS are found to be stable in the NaCl structure, and ThBi and ThTe in the CsCl structure, for pressures below 50 GPa. The electronic structures of the ThX compounds are studied using the quasiparticle self-consistent GW method (G: Green function, W: dynamically screened interaction).

General information
State: Published
Organisations: Department of Physics, University of Hyderabad, Aarhus University, European Commission - Joint Research Center, University of Copenhagen, Indian Institute of Technology Hyderabad
Contributors: Kanchana, V., Vaitheeswaran, G., Svane, A., Heathman, S., Gerward, L., Olsen, J. S.
Number of pages: 10
Pages: 459-468
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Acta Crystallographica. Section B: Structural Science
Volume: 70
Issue number: 3
ISSN (Print): 0108-7681
Ratings:
Web of Science (2018): Indexed yes
Scopus rating (2017): CiteScore 4.54 SJR 1.654 SNIP 1.604
Web of Science (2017): Impact factor 6.467
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.14 SJR 0.675 SNIP 1.002
Web of Science (2016): Impact factor 2.032
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.37 SJR 0.86 SNIP 1.482
Web of Science (2015): Impact factor 2.892
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.94 SJR 0.846 SNIP 2.467
Web of Science (2014): Impact factor 2.184
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.68 SNIP 0.969
Web of Science (2013): Impact factor 2.095
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.942 SNIP 1.392
Web of Science (2012): Impact factor 2.175
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.916 SNIP 1.395
Web of Science (2011): Impact factor 2.286
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1