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Thermal expansion of ScF_3: insights from density-functional molecular dynamics in the isothermal-isobaric ensemble

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Negative thermal expansion (NTE) of materials is an unusual and interesting phenomenon as most materials expand upon heating. Technological applications related to the NTE phenomenon are enormous [1]: from dental fillings to high precision optical mirrors, fuel cells, and thermoelectric converters. Most of the materials exhibiting the NTE have complex structure with low-symmetry which complicates a detailed understanding of the NTE phenomenon but recently [2], a large and isotropic NTE over a broad range of temperatures has been observed in compound ScF_3 with a cubic structure. In my contribution, I will report on our recent work [3], in which we studied the thermal behavior of ScF_3 by means of density functional theory in connection with molecular dynamics in the isothermal-isobaric ensemble. I will show that our simulations reproduce the experimentally observed trends [2] (i.e. negative thermal expansion at low temperatures, nearly zero expansion at ~1000 K, and positive expansion at higher temperatures). An atomistic scenario of the observed phenomena will be analyzed and a strong connection between thermal expansion and instantaneous rhombohedral distortions of the cubic cell resulting from the thermal motion of atoms will be demonstrated.

[1] K. Takenaka, Sci. Technol. Adv. Mater. 13 (2012) 013001.

[2] B. K. Greve, K. L. Martin, et al., J. Am. Chem. Soc. 132 (2010) 15496.

[3] P. Lazar, T. Bučko, J. Hafner, Phys. Rev. B 92 (2015) 224302.

Jeudi 7 juillet 2016 à 15 h 00

Salle Réunion Chimie – I.C.P.M.

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