Finding better materials faster: The example of magnetocalorics

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Abstract

I will describe a new effort to seek out exciting new room-temperature magnetocaloric materials. The material property of interest in finding candidate magnetocaloric materials is their gravimetric entropy change upon application of a magnetic field under isothermal conditions. We have proposed a simple computational proxy based on carrying out non-magnetic and magnetic density functional theory calculations on magnetic materials. This proxy, which we refer to as the magnetic deformation $\Sigma M$, is a measure of how much the unit cell deforms when comparing the relaxed structures with and without the inclusion of spin polarization. $\Sigma M$ appears to correlate very well with experimentally measured magnetic entropy change values.[1]


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Ram Seshadri is the Fred and Linda R. Wudl Professor of Materials Science at UC Santa Barbara. He is also a Professor in the Department of Chemistry and Biochemistry. He received his PhD in Solid State Chemistry in 1995 from the Indian Institute of Science, Bangalore, and after some years as a postdoctoral fellow in Europe, returned to Bangalore as an Assistant Professor in 1999. He moved to UC Santa Barbara in 2002. At UCSB, he also serves as the Director of the Materials Research Laboratory: A National Science Foundation Materials Research Science and Engineering Center (NSF-MRSEC). His research work, embodied in 300+ publications, addresses the topic of structure-property relations in crystalline inorganic materials, with a focus on materials for energy applications. He is a Fellow of the Royal Society of Chemistry, and of the American Physical Society. He has served on the Editorial Committee of Annual Reviews of Materials Research since 2008, and as an Associate Editor of Chemistry of Materials since 2015.