

Abstract Submitted
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Computational search for rare-earth free hard-magnetic materials¹ JOSÉ A. FLORES LIVAS, SANGEETA SHARMA, JOHN KAY DEWHURST, EBERHARD GROSS, Max Planck Inst Microstructure, MAGMAT TEAM — It is difficult to over state the importance of hard magnets for human life in modern times; they enter every walk of our life from medical equipments (NMR) to transport (trains, planes, cars, etc) to electronic appliances (for house hold use to computers). All the known hard magnets in use today contain rare-earth elements, extraction of which is expensive and environmentally harmful. Rare-earths are also instrumental in tipping the balance of world economy as most of them are mined in limited specific parts of the world. Hence it would be ideal to have similar characteristics as a hard magnet but without or at least with reduced amount of rare-earths. This is the main goal of our work: search for rare-earth-free magnets. To do so we employ a combination of density functional theory and crystal prediction methods. The quantities which define a hard magnet are magnetic anisotropy energy (MAE) and saturation magnetization (Ms), which are the quantities we maximize in search for an ideal magnet. In my talk I will present details of the computation search algorithm together with some potential newly discovered rare-earth free hard magnet.

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