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Nuclear Magnetic Resonance Chemical Shielding Calculations of Bulk Oxides[1] DANIEL PECHKIS[2], ERIC J. WALTER, HENRY KRAKAUER, College of William and Mary — We will present calculations of nuclear magnetic resonance (NMR) chemical shielding in oxides, modeled using embedded clusters. NMR spectroscopy is an important probe of local structure in disordered materials, such as ferroelectric perovskite solid solutions. Combined with electric field gradient (EFG) calculations, a complete interpretation of high magnetic field NMR spectra is possible in principle. Determination of NMR parameters within the embedded cluster method allows the study of both periodic and disordered systems. Moreover, this approach can take advantage of mature chemical shielding methods found in standard quantum chemistry electronic structure packages at several levels of theory, including different forms of density functionals as well as more correlated approaches. Results will be presented for several materials including ferroelectric perovskites.

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Daniel Pechkis
College of William and Mary

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