Electric field gradients in embedded cluster calculations

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Electric field gradients (EFGs) at atomic nuclei provide a sensitive probe of the local electronic structure and symmetry of solids. In this contribution, we present a methodology for the calculation of EFGs in solids using embedded-cluster method. In particular, we demonstrate its application to ^{229}Th-doped calcium fluoride (CaF_2:Th) [1,2]. As EFGs determine the quadrupole splitting of the low-energy nuclear states of ^{229}Th, they are a key parameter in the development of solid-state nuclear clocks. We discuss the results in the context of recent Mössbauer spectroscopy experiments that demonstrated the existence of several distinct thorium sites in CaF_2 [3,4].

[1] A. Derevianko et al. https://arxiv.org/pdf/2601.07098
[2] K. Nalikowski et al. Phys. Rev. B 111 (2025) 115103
[3] T. Hiraki et al. https://arxiv.org/pdf/2509.00041
[4] T. Ooi et al. Nature 650 (2026) 72

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