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First-principles calculations of Ti and O NMR chemical shift tensors in ferroelectric perovskites[1] DANIEL PECHKIS, ERIC WALTER, HENRY KRAKAUER, College of William and Mary — Complementary chemical shift calculations were carried out with embedded clusters, using quantum chemistry methods, and with periodic boundary conditions, using the GIPAW approach[2] within the Quantum Espresso package.[3] Compared to oxygen chemical shifts, $\hat{\delta}$(O),[4] cluster calculations for $\hat{\delta}$(Ti) were found to be more sensitive to size effects, termination, and choice of gaussian-type atomic basis set, while GIPAW results were found to be more sensitive to the pseudopotential construction. The two approaches complemented each other in optimizing these factors. We show that the two approaches yield comparable chemical shifts for suitably converged simulations, and results are compared with available experimental measurements.

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[3]P. Giannozzi et al., Journal of Physics: Condensed Matter **21**, 395502 (2009)
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