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All−electron magnetic response with pseudopotentials: NMR chemical shifts

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A theory for the *ab initio* calculation of the all−electron magnetic response in insulators using pseudopotentials is presented. It is formulated for both finite and infinitely periodic systems and is based on an extension to the Projector Augmented Wave approach of Blöchl [P. E. Blöchl, Phys. Rev. B **50**, 17953 (1994)] and the method of Mauri *et al* [F. Mauri, B. G. Pfrommer, and S. G. Louie, Phys. Rev. Lett. **77**, 5300 (1996)]. The theory is applied to the calculation of NMR chemical shifts in a variety of systems.
