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NMR chemical shifts from first-principles using the converse approach in periodic boundary conditions DAVIDE CERESOLI, TIMO THONHAUSER, MIT, NICOLA MARZARI — An alternative, converse approach to the first-principles calculation of NMR shielding tensors can be formulated where NMR chemical shift are obtained from the derivative of the orbital magnetization with respect to the application of a microscopic, localized magnetic dipole. We apply here the modern theory of orbital magnetization to validate this formalism to the case of extended systems in periodic boundary conditions, finding very good agreement with established methods and experimental results. These results underscore the advantages of the converse approach over existing methods: (1) it can be applied to either isolated or periodic systems, (2) it avoids any linear response calculation, allowing to treat systems containing hundreds of atoms, and (3) it is not plagued by the gauge-origin problem.

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