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***Ab Initio* Theory of Nuclear Magnetic Resonance Shifts in Metals** MAYEUL D'AVEZAC, Laboratoire de Mineralogie-Cristallographie de Paris, NICOLA MARZARI, Department of Materials Science and Engineering, MIT, FRANCESCO MAURI, Laboratoire de Mineralogie-Cristallographie de Paris — A comprehensive approach for the first-principles determination of all-electron NMR shifts in metallic systems is presented. Our formulation is based on a combination of density-functional perturbation theory and all-electron wavefunction reconstruction, starting from periodic-boundary calculations in the pseudopotential approximation. The orbital contribution to the NMR shift (the chemical shift) is obtained by combining the gauge-including projector augmented-wave approach (GIPAW), originally developed for the case of insulators[1], with the extension of linear-response theory to the case of metallic systems[2]. The spin contribution (the Knight shift) is obtained as a response to a finite uniform magnetic field, and through reconstructing the hyperfine interaction between the electron-spin density and the nuclear spins with the projector augmented-wave method (PAW[3]). Our method is validated with applications to the case of the homogeneous electron gas and of simple metals. (Work supported by MURI grant DAAD 19-03-1-0169 and MIT-France)

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