Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

A Converse Approach to NMR Chemical Shifts for Norm-Conserving Pseudopotentials GRAHAM LOPEZ, Wake Forest University, DAVIDE CERESOLI, NICOLA MARZARI, Massachusetts Institute of Technology, TIMO THONHAUSER, Wake Forest University — Building on the recently developed converse approach for the ab-initio calculation of NMR chemical shifts [1], we present a corresponding framework that is suitable in connection with norm-conserving pseudopotentials. Our approach uses the GIPAW transformation [2] to set up a formalism where the derivative of the orbital magnetization [3] is taken with respect to a microscopic, localized magnetic dipole in the presence of pseudopotentials. The advantages of our method are that it is conceptually simple, the need for a linear-response framework is avoided, and it is applicable to large systems. We present results for calculations of several well-studied systems, including the carbon, hydrogen, fluorine, and phosphorus shifts in various molecules and solids. Our results are in very good agreement with both linear-response calculations and experimental results.

[1] T. Thonhauser et al., J. Chem. Phys. **131**, 101101 (2009).
[2] C. J. Pickard and F. Mauri, Phys. Rev. B **63**, 245101 (2001).
[3] T. Thonhauser et al., Phys. Rev. Lett. **95**, 137205 (2005).

Graham Lopez
Wake Forest University

Date submitted: 16 Nov 2009 Electronic form version 1.4