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How First-Principles Calculations Combined with ^{95}Mo Solid-State NMR Can Help in the Understanding of Inorganic Materials?

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Since the 1980s, the expansion of solid-state NMR has increased significantly owing to the development of new techniques that enable high resolution to be achieved even in the solid state. For inorganic compounds without protons or fluorine atoms, the two dominant interactions responsible for the appearance of the NMR spectrum are the chemical shift anisotropy and the quadrupolar interaction tensors. These parameters give information about the atomic structure of the compound under investigation. It appears that in many cases, the complexity of the experimental results require a theoretical analysis for their complete understanding. Until recently, only quadrupolar interaction parameters could be calculated using periodic DFT calculations. Pickard and Mauri presented a formalism, named GIPAW, for the *ab initio* calculation of all-electron NMR chemical shifts in insulators using pseudopotentials.[1]

We present the combined application of ^{95}Mo solid-state NMR and DFT calculations for the study of materials such as molybdenum cluster compounds and nanoparticles.[2] The power of this combined approach for the investigation of solid-state materials will be shown as well as its limitations.[3]

1 C. J. Pickard, F. Mauri *Phys. Rev. B* **2001**, *63*, 245101.
2 *Nanoparticles. From Theory to Applications*, ed. G. Schmid, Wiley-VCH, **2010**.
3 See for example: (a) J. Cuny, S. Messaoudi, V. Alonzo, E. Furet, J.-F. Halet, E. Le Fur, S. E. Ashbrook, C. J. Pickard, R. Gautier, L. Le Pollès *J. Comput. Chem.* **2008**, *29*, 2279 (b) J. Cuny, E. Furet, R. Gautier, L. Le Pollès, C. J. Pickard, J.-B. d'Espinose de Lacaillerie *ChemPhysChem* **2009**, *10*, 3320. (c) P. Gougeon, D. Salloum, J. Cuny, L. Le Pollès, M. Le Floch, R. Gautier, M. Potel *Inorg. Chem.* **2009**, *48*, 8337.

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