Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Quantum pressure in molecules and solids: Influence of magnetic fields and spin-orbit coupling on electron localization[1] JIANMIN TAO, SHI LIU, FAN ZHENG, ANDREW M. RAPPE, University of Pennsylvania — The most important concept in chemistry is chemical bond, which has been used by chemists to explain the properties of molecules and solids as well as chemical processes. Considerable efforts [1,2] have been made toward a simple and yet fundamental understanding of this concept. Here we formulate the quantum pressure in an external magnetic field, allowing us to study the influence of magnetic fields and spin-orbit coupling on electron localization in molecules and solids. We find that electrons in conjugated molecules become more localized in strong magnetic fields, due to the induced currents. We demonstrate that the quantum pressure not only can reveal electronic shell structures of atoms [3], but also can be used to visualize bonding structures of molecules and solids, significantly extending the applicability of this descriptive tool.

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[1]This work was supported by NSF, USAF, and DOE

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Date submitted: 14 Nov 2014 Electronic form version 1.4