Getting to Lewis electron pairs from quantum mechanical calculations: Maximum Probability Domains

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A method is presented to recover Lewis' picture from quantum mechanical calculations[1]: a spatial domain is defined by maximizing the probability to find a pair of electrons in it. This definition has not only the advantage of simplicity. It can be applied to any type of wave function (examples: Hartree-Fock, or correlated with Jastrow factors)[2]. It does not only recover Lewis' picture in trivial organic molecules, but also in crystals. In the same spirit, other questions can be asked, beyond the electron pair concept, e.g., identifying ions[3].

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[2] Scemama A., Caffarel M., Savin A., *J. Comp. Chem.* 28:442, 2007.

[3] Causà M., Savin A., *J. Phys. Chem. A* 115:13139, 2011.