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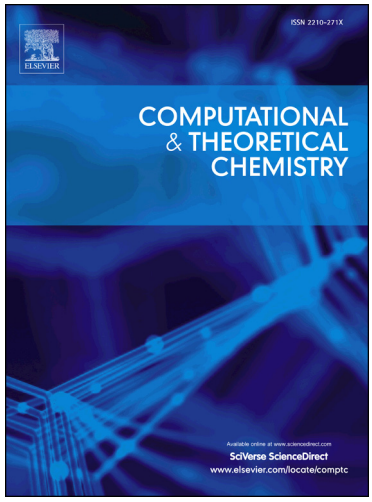

Bond metallicity measures

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ACCEPTED MANUSCRIPT

Bond Metallicity Measures

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It was recently proposed that the metallicity of chemical bond can be determined by the electron density divided by its Laplacian, evaluated at the bond critical point, $\rho(\mathbf{r}_{bcp})/\nabla^2\rho(\mathbf{r}_{bcp})$. We define a new, dimensionless, form of this bond metallicity measure. We explain why these bond metallicity measures work by showing that the bond metallicity is inversely related to "nearsightedness" of the first-order density matrix. These bond metallicity measures are also related to various measures of electron localization functions and atomic shell structure that have been proposed in the literature. The local electronic temperature provides a common basis for understanding the links between most of the electron localization measures that appear in the literature. High local temperature is associated with nearsightedness of the first-order density matrix, high electron localization, and small values of our bond metallicity measures.

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