

Theoretical studies of mixed-valence organometallic species for potential utilization as quantum cellular automata

Thomas Groizard, Samia Kahlal, Jean-François Halet*

Institut des Sciences Chimiques de Rennes, UMR 6226 CNRS-Université de Rennes 1, Avenue du Général Leclerc, F-35042 Rennes Cédex, France

Supplementary Information

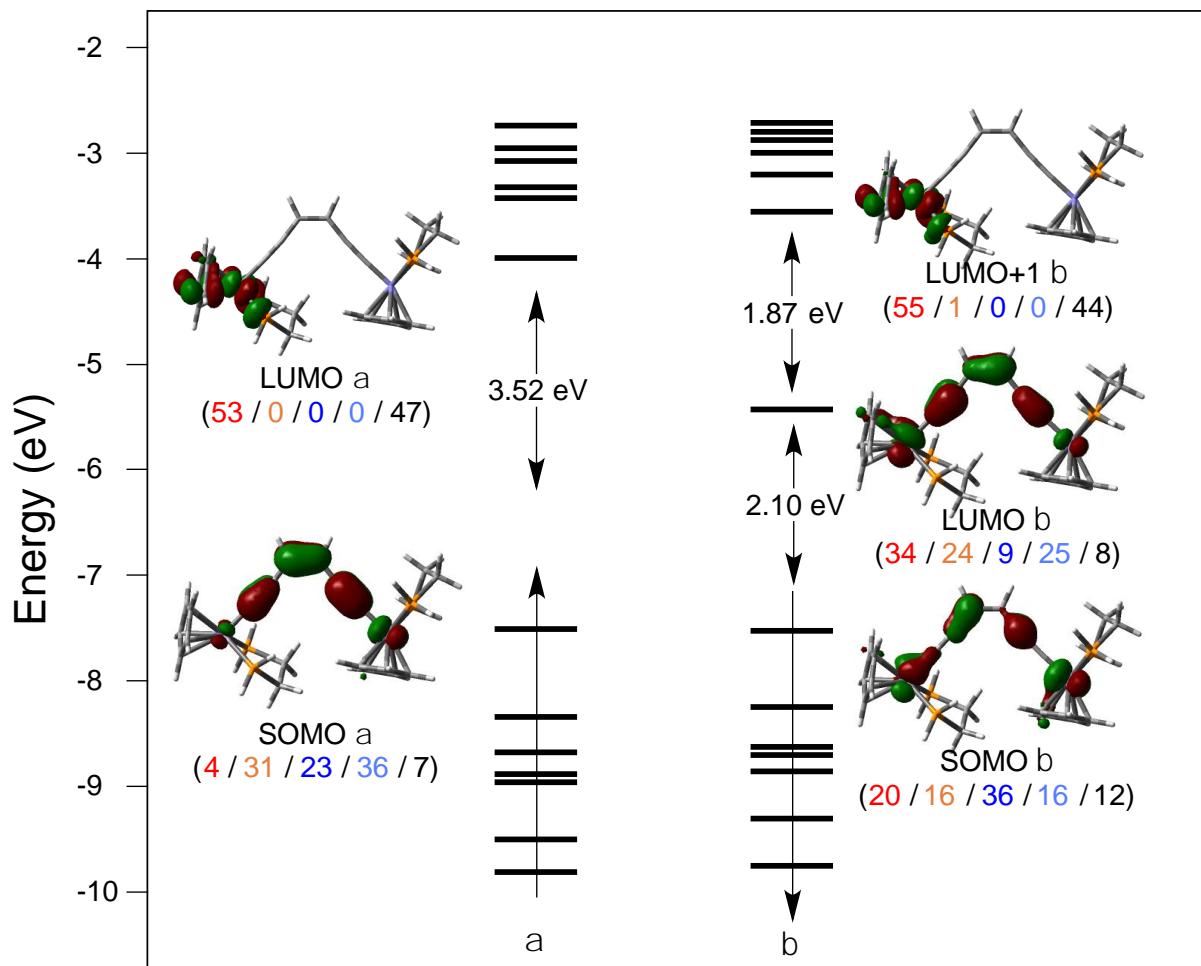


Figure S1. Spin orbital diagram of 16-H^+ . The Fe(1)/left carbon chain/Fe(2)/right carbon chain/Cp* and dppe percentage contributions are given in brackets. Contour values are ± 0.04 ($e \text{ bohr}^{-3}\right)^{1/2}$.

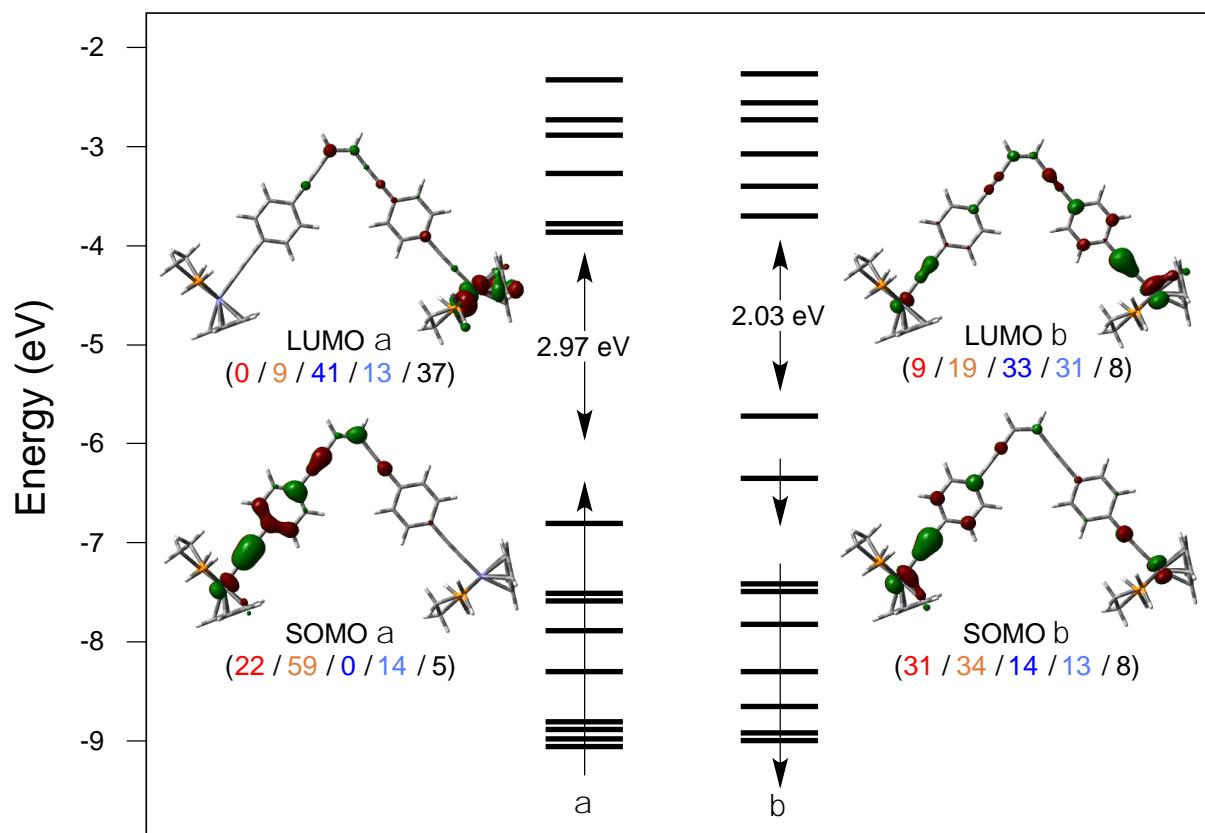


Figure S2. Spin orbital diagram of $\mathbf{17}\text{-H}^+$. The Fe(1)/left carbon chain/Fe(2)/right carbon chain/Cp* and dppe percentage contributions are given in brackets. Contour values are ± 0.04 ($e\text{ bohr}^{-3}\right)^{1/2}$.