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Electronic Supplementary Information

Quantum Chemical and Experimental Insights for the Ionic Liquid Facilitated Thermal Dehydrogenation of Ethylene Diamine Bisborane

Basudhrity Banerjee, Debashis Kundu, G. Pugazhenthi and Tamal Banerjee*

Department of Chemical Engineering, Indian Institute of Technology Guwahati, Assam, India 781039

Table S1. COSMO-SAC parameters

COSMO-SAC parameters	**Values**
Effective area (a_{eff})	6.32 Å^2
Coefficient of hydrogen bonding (C_{hb})	75006 (Kcal Å^4)/(mol e^2)
Hydrogen bonding cut off (σ_{hb})	0.0084 e/Å^2
Permittivity in free space (ε_0)	2.395x10^{-4} (e^2 mol)/(kcal Å)

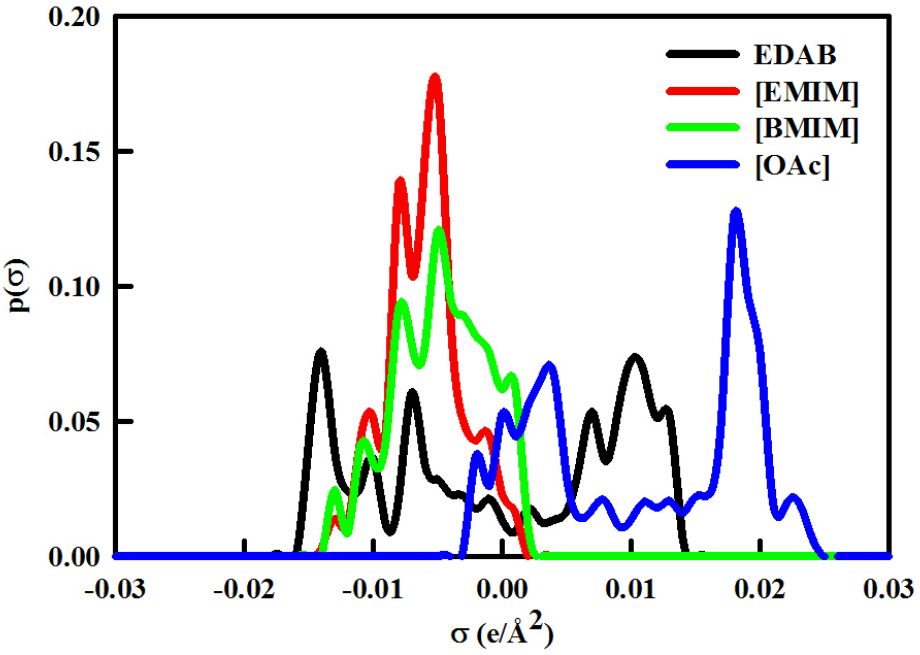

Fig. S1. σ-profile of EDAB, imidazolium cations and acetate anions.

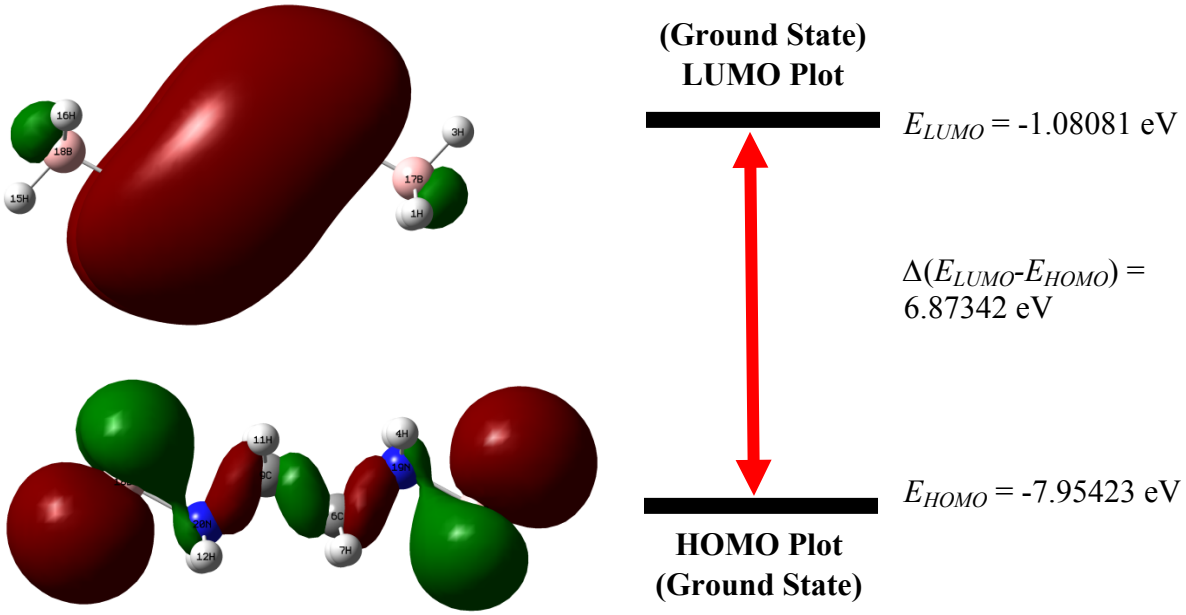

Fig. S2. LUMO-HOMO energy gap of EDAB

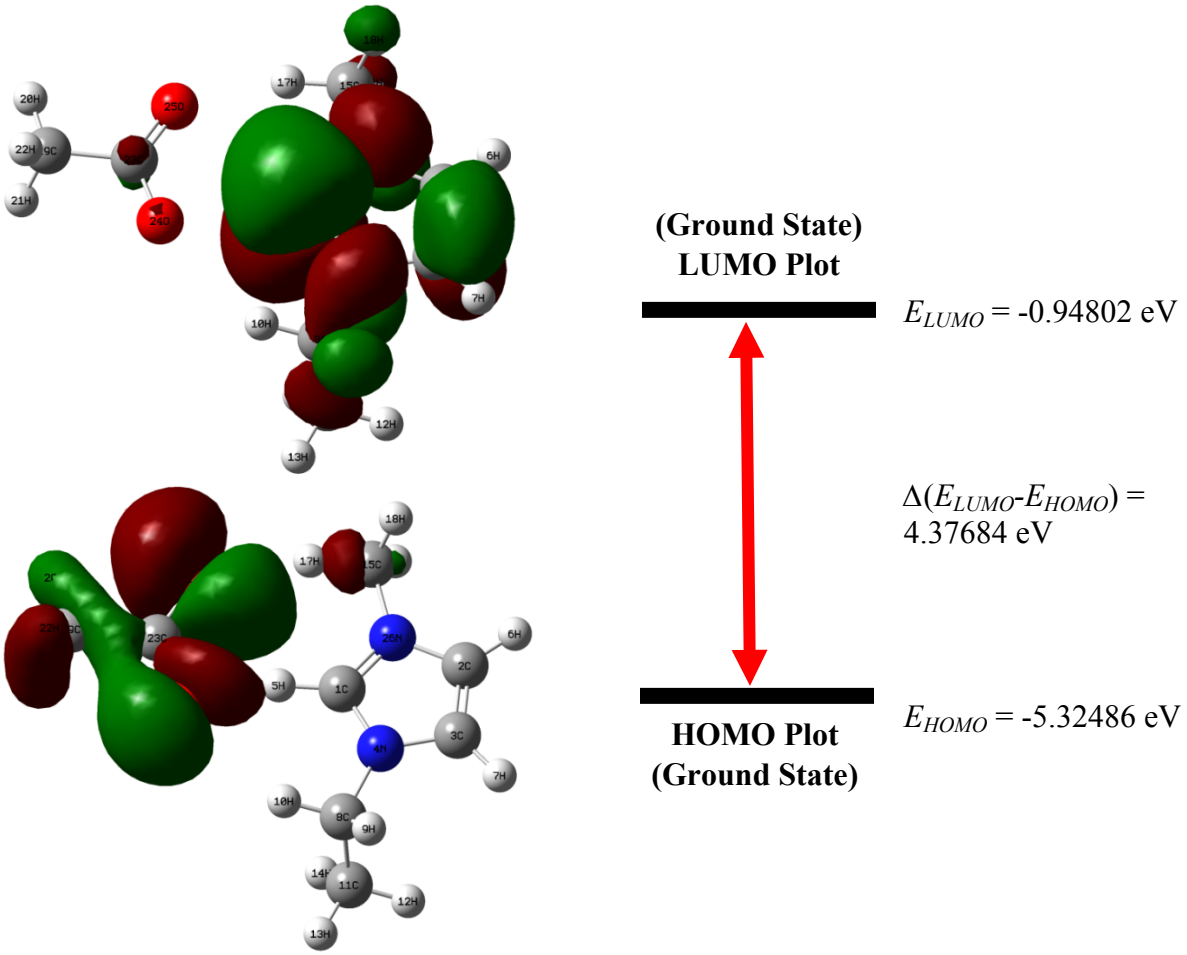

Fig. S3. LUMO-HOMO energy gap of [EMIM][OAc]

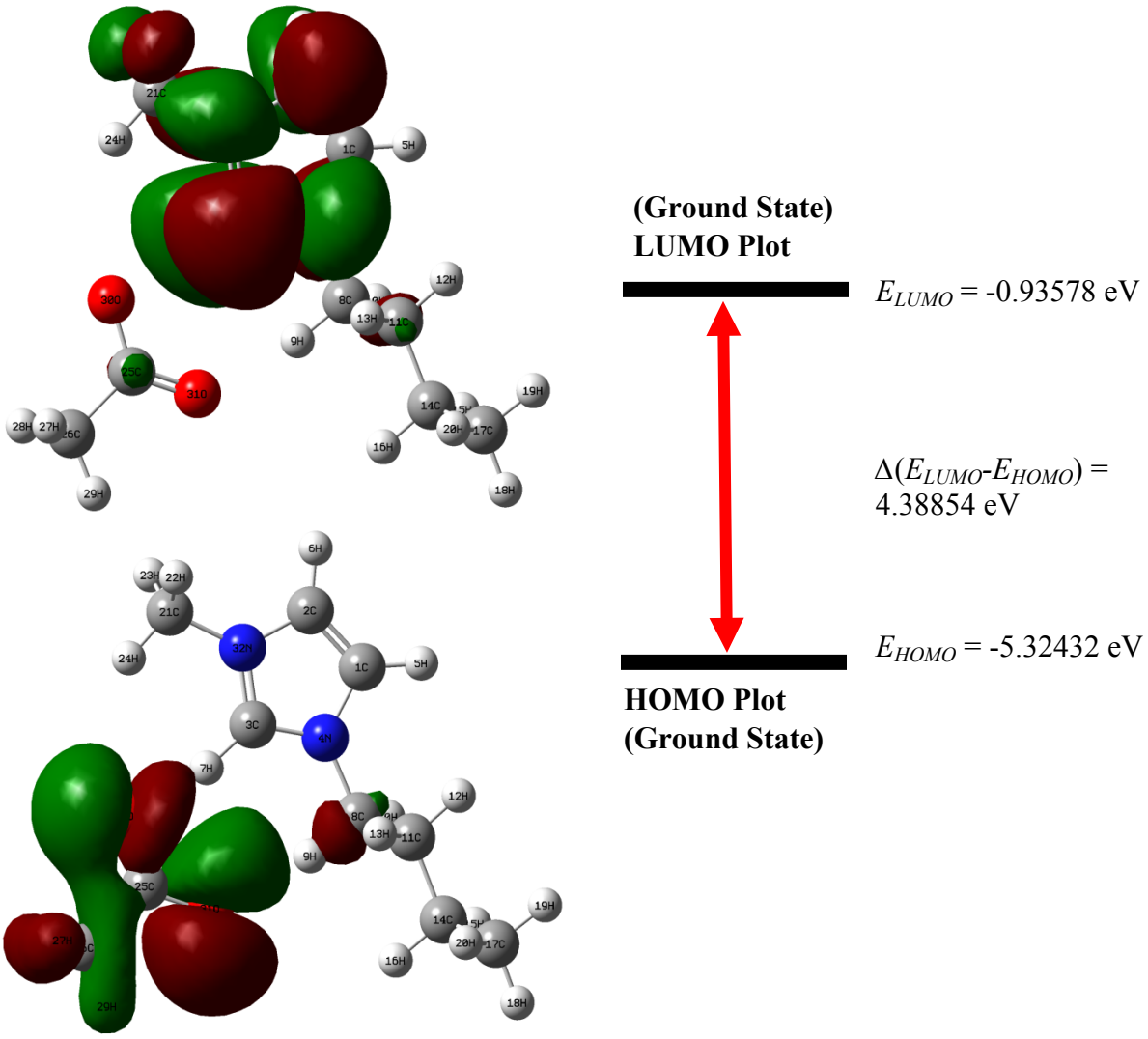

Fig. S4. LUMO-HOMO energy gap of [BMIM][OAc]