Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Site-specific electronic structure of imidazole and imidazolium in aqueous solutions

F. Meyer[1], M. Blum[2], A. Benkert[1,3], D. Hauschild[1,3,4], Y.L. Jeyachandran[5], R.G. Wilks[6], W. Yang[7], M. Bär[6], F. Reinert[1], C. Heske[2,3,4], M. Zharnikov[5], and L. Weinhardt[2,3,4*]

[1]*Universität Würzburg, Experimentelle Physik VII, Am Hubland, 97074 Würzburg, Germany*

[2] *Department of Chemistry and Biochemistry, University of Nevada, Las Vegas (UNLV), 4505 Maryland Parkway, NV 89154-4003, USA*

[3]*Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology (KIT), Hermann-v.-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany*

[4]*Institute for Chemical Technology and Polymer Chemistry (ITCP), Karlsruhe Institute of Technology (KIT), Engesserstr. 18/20, 76128 Karlsruhe, Germany*

[5]*Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany*

[6]*Renewable Energy, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany*

[7]*Advanced Light Source (ALS), Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720, USA*

*corresponding author: lothar.weinhardt@kit.edu

	Calculated Orbital Energy (eV)	
	Imidazole (Im)	Imidazolium (ImH^+)
LUMO+2	0.58	-4.36
LUMO+1	0.36	-5.79
LUMO	-0.61	-6.89
HOMO	-5.81	-11.97
HOMO-1	-6.31	-13.77
HOMO-2	-6.98	-16.39

Table S1: Calculated orbital energies (in eV).

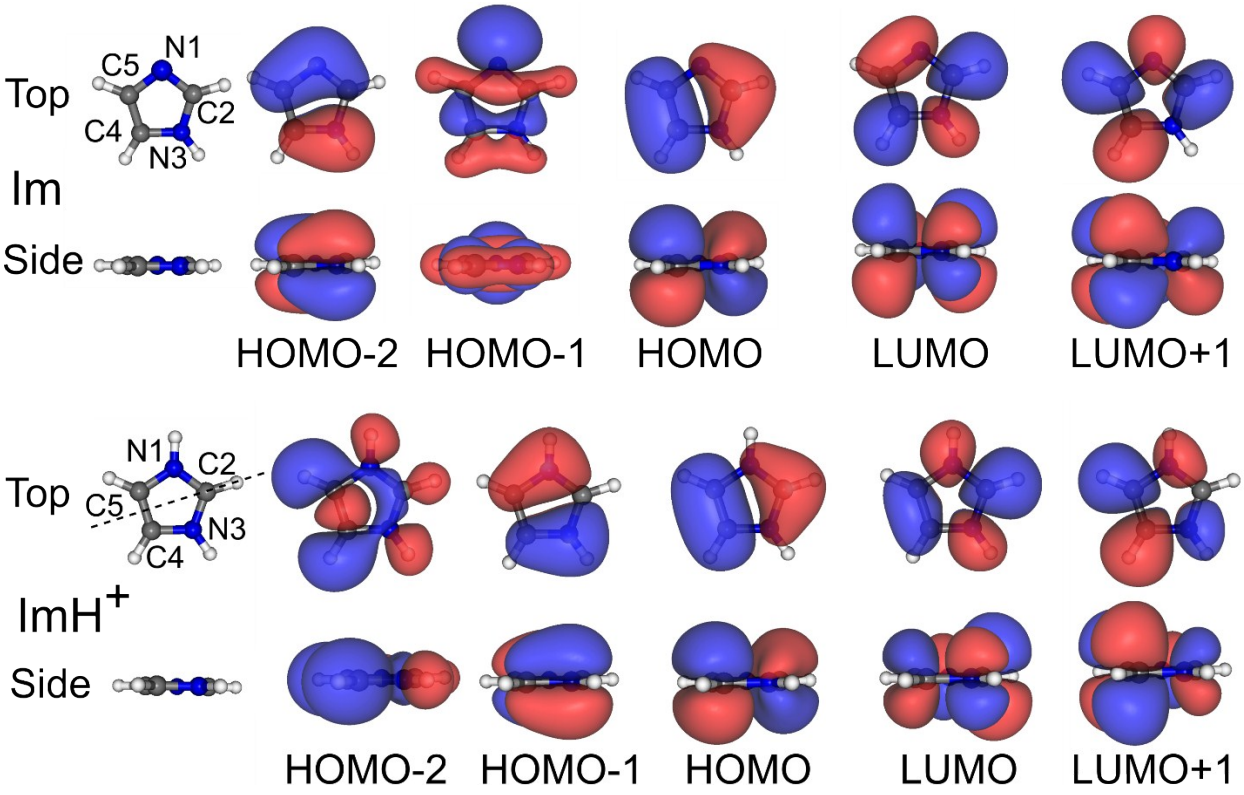

Figure S1: Calculated isodensity surfaces of the three highest occupied and two lowest unoccupied molecular orbitals of Im (top) and ImH^+ (bottom), respectively (isosurface value: $\pm 0.02 \frac{e}{a_0^3}$).