

Description of Additional Supplementary Files

Supplementary Data 1. ESP: HVOC.txt, MVOC.txt.

Supplementary Data 2. Adsorption energies: HVOC-I-.txt, HVOC-I2.txt, HVOC-I3.txt, HVOC-I5.txt, MVOC-I-.txt, MVOC-I2.txt, MVOC-I3.txt, MVOC-I5.txt.

Supplementary Data 3. Charge density difference: HVOC-I3.txt, HVOC-I5.txt.

Supplementary Data 4. MD of BE and HVOC: BE.txt, HVOC.txt.

Supplementary Data 5. MD of BE and HVOC: BE.txt, HVOC.txt.

Supplementary Data 6. Gibbs free energy: HVOC-I-.txt, HVOC-I2.txt, HVOC-I3.txt, HVOC-I5.txt, MVOC-I-.txt, MVOC-I2.txt, MVOC-I3.txt, MVOC-I5.txt.

Supplementary Data 7. Binding energies: HVOC-OTF.txt, Zn-OTF.txt; MD of HVOC: HVOC.txt

Supplementary Data 8. Reduction potentials: F-.txt, OTF.txt, SO3.txt, SO3CF2.txt, ZnCF3.txt, ZnF2.txt, Zn-OTF.txt.

Supplementary Data 9. Binding energy: ZnF2-Zn.xsd, ZnS-Zn.xsd, Zn-Zn.xsd.

Supplementary Data 10. ESP: I-.txt, I2.txt, I3.txt, I5.txt.

Supplementary Data 11. Orbital energy: HVOC.txt, I-.txt, I2.txt, I3.txt, I5.txt, MVOC.txt, OTF.txt.

Supplementary Data 12. Charge density difference: HVOC-I-.LOG, HVOC-I-.fchk.

Supplementary Data 13. MD of BE, HVOC, MVOC.