Supporting Information: A tight-binding approach to pyrazine-mediated superexchange in copper-pyrazine antiferromagnets

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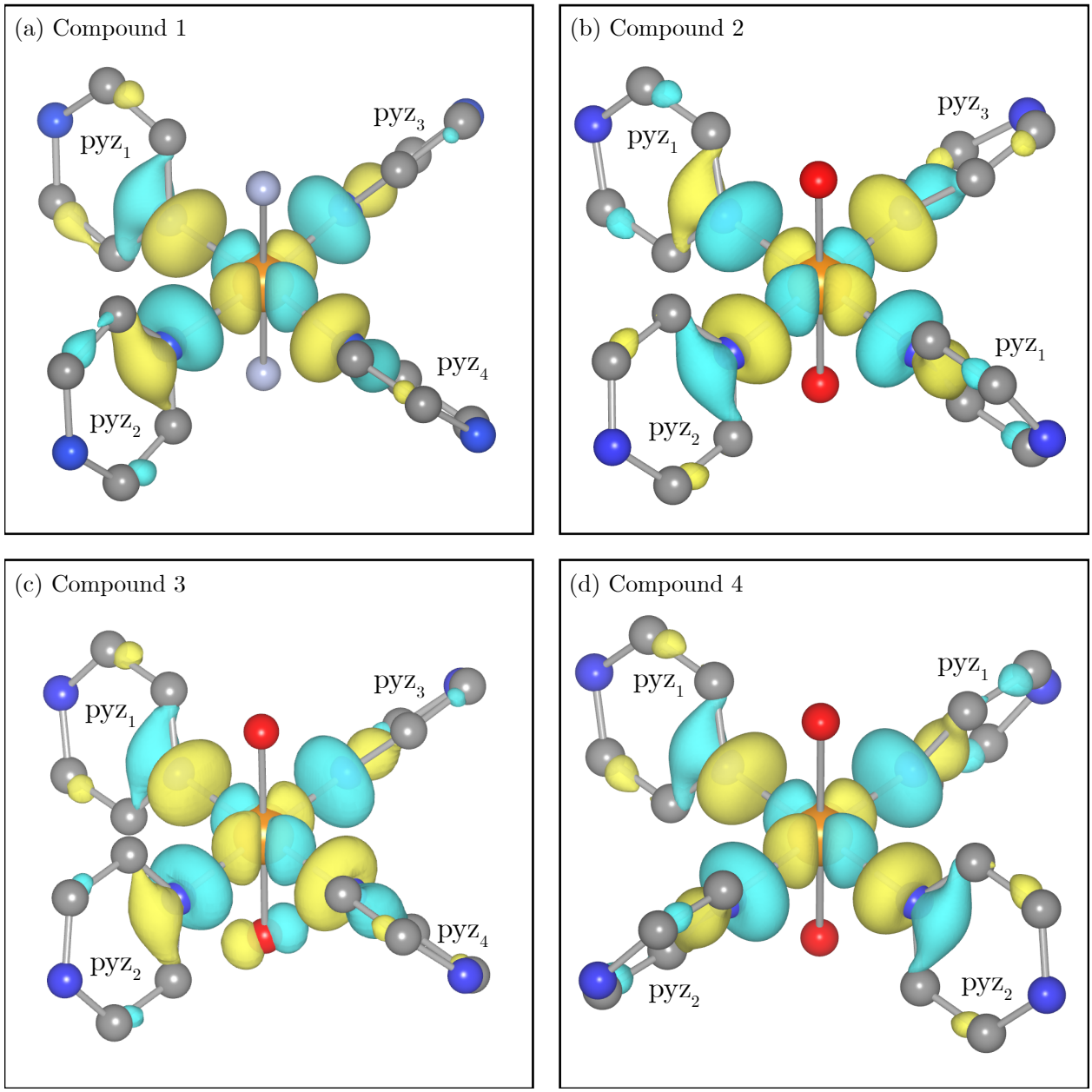

Figure S1: Cu-centered Wannier functions for the two-Wannier model (one on each Cu in the unit cell) for (a) **1**, (b) **2**, (c) **3**, and (d) **4**. All resemble hybrid orbitals of Cu $d_{x^2-y^2}$ and N sp^2. In **3**, there is some weight on one of the inter-layer ligands, 4-phpy-O.

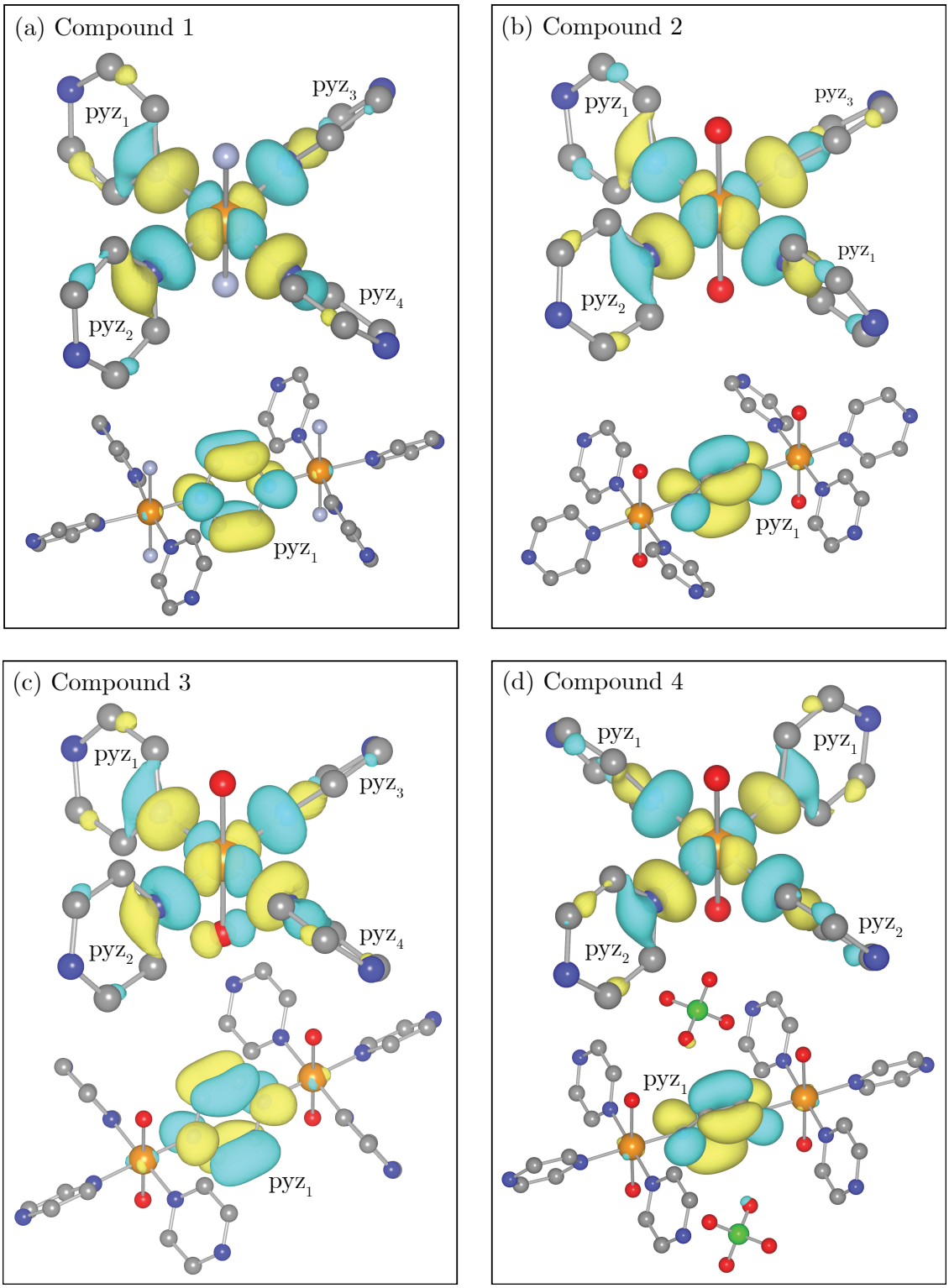

Figure S2: Cu-centered and pyz-centered Wannier functions for the six-Wannier model (one on each Cu and pyz in the unit cell) for (a) **1**, (b) **2**, (c) **3**, and (d) **4**. All Cu-centered functions are very similar to their counterparts in the two-Wannier model (in Figure S1). The pyz-centered Wanniers all resemble the lowest, unoccupied molecular orbital of an isolated pyz. The other pyz-centered functions (not shown here) are all similar to the ones shown.