

Abstract Submitted  
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**Accurate potential energy surfaces for transition-metal complexes with DFT+ $U(\mathbf{R})$**  HEATHER KULIK, Stanford University — We introduce an improvement to the Hubbard  $U$  augmented density functional approach known as DFT+ $U$  that incorporates variations in the value of self-consistently calculated, linear-response  $U$  with changes in geometry. This approach overcomes the one major shortcoming of previous DFT+ $U$  studies, i.e. the use of an averaged Hubbard  $U$  when comparing energies for different points along a potential energy surface is no longer required. While DFT+ $U$  is quite successful at providing accurate descriptions of localized electrons (e.g.  $d$  or  $f$ ) by correcting self-interaction errors of standard exchange correlation functionals, we show several examples from diatomic molecules to porphyrins to surface science applications where this position-dependent DFT+ $U(\mathbf{R})$  provides a significant two- to four-fold improvement over DFT+ $U$  predictions. DFT+ $U(\mathbf{R})$  reduces errors in binding energies, frequencies, and equilibrium bond lengths by applying the linear-response, position-dependent  $U(\mathbf{R})$  at each point. We also propose a metric for whether a standard DFT+ $U$  approach is sufficient by determining the strength of the dependence of  $U$  on changes in coordinates.

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