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Rethinking CO adsorption on transition-metal surfaces: Effect of density-driven self-interaction errors

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#	Paper	IF	Citations
38	Toward a First-Principles Evaluation of Transport Mechanisms in Molecular Wires. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 6267-6279	6.4	2
37	Density Functional Theory for Molecule-Metal Surface Reactions: When Does the Generalized Gradient Approximation Get It Right, and What to Do If It Does Not. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 10552-10560	6.4	20
36	Application of accelerated long-range corrected exchange functional [LC-DFT(2Gau)] to periodic boundary condition systems: CO adsorption on Cu(111) surface. <i>Journal of Chemical Physics</i> , <b>2020</b> , 152, 104105	3.9	1
35	BaZrO <sub>3</sub> stability under pressure: The role of nonlocal exchange and correlation. <i>Physical Review B</i> , <b>2020</b> , 101,	3.3	4
34	CO, NO, and SO adsorption on Ni nanoclusters: a DFT investigation. <i>Dalton Transactions</i> , <b>2020</b> , 49, 6407-6417	4.5	12
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32	Computational approaches to dissociative chemisorption on metals: towards chemical accuracy. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 8962-9048	3.6	26
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24	vdW-DF-ahcx: a range-separated van der Waals density functional hybrid. <i>Journal of Physics Condensed Matter</i> , <b>2021</b> , 34,	1.8	2
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21	Large vibrational free energy of tightly bonded small chemicals on metal surfaces. <i>Applied Surface Science</i> , <b>2021</b> , 575, 151778	6.7	0
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- 2 Spin-state gaps and self-interaction-corrected density functional approximations: Octahedral Fe(II) complexes as case study. **2023**, 158, 054305 ○
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