Supplementary Materials for

"Effect of spin contamination error and importance of open-shell structure for aggregation of Au atoms on a MgO surface"

Kohei Tada [1,*], Tomohiro Maruyama [2], Hiroaki Koga [3], Mitsutaka Okumura [2,3], and Shingo Tanaka [1]

[1] Department of Energy and Environment, National Institute of Advanced Industrial Science and Technology (AIST), 1-8-31, Midorigaoka, Ikeda, Osaka, 563-8577, Japan

[2] Department of Chemistry, Graduate School of Science, Osaka University,1-1, Machikaneyama, Toyonaka, Osaka, 560-0043, Japan

[3] Elements Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University, 1-30 Goryo Ohara, Nishikyo, Kyoto, Kyoto 615-8245, Japan

* Corresponding Author

phone: +81-72-751-8566

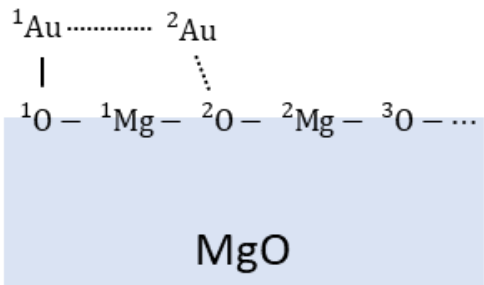fax: +81-72-751-9714

k-tada@aist.go.jp

Contents

Captions for Table S1 and Figure S1

Table S1   The nearest neighbor atoms of the ^{2}Au atom for all r.

Figure S1. Spin density distributions of the HS states. Isosurface values are 0.004 e/Bohr^3.

Table S1 The nearest neighbor atoms of the ^{2}Au atom for all r.

r	LS	HS	BS
0.000	^{1}Au	^{1}Au	^{1}Au
0.025	^{1}Au	^{1}Au	^{1}Au
0.050	^{1}Au	^{1}Au	^{1}Au
0.075	^{1}Au	^{1}Au	^{1}Au
0.100	^{1}Au	^{1}Au	^{1}Au
0.125	^{1}Au	^{1}Au	^{1}Au
0.150	^{1}Au	^{1}Au	^{1}Au
0.175	^{1}Mg	^{1}Mg	^{1}Mg
0.200	^{2}O	^{2}O	^{2}O
0.225	^{2}O	^{2}O	^{2}O
0.250	^{2}O	^{2}O	^{2}O
0.275	^{2}O	^{2}O	^{2}O
0.300	^{2}O	^{2}O	^{2}O
0.325	^{2}Mg	^{2}Mg	^{2}Mg
0.350	^{2}Mg	^{2}Mg	^{2}Mg
0.375	^{2}Mg	^{2}Mg	^{2}Mg
0.400	^{2}Mg	^{2}Mg	^{2}Mg
0.425	^{2}Mg	^{2}Mg	^{2}Mg
0.450	^{3}O	^{3}O	^{3}O
0.475	^{3}O	^{3}O	^{3}O
0.500	^{3}O	^{3}O	^{3}O

^{1}Au ‑‑‑‑‑‑‑‑ ^{2}Au

^{1}O – ^{1}Mg – ^{2}O – ^{2}Mg – ^{3}O – ⋯

MgO

r = 0.000   r = 0.025   r = 0.050   r = 0.075

r = 0.100   r = 0.125   r = 0.150   r = 0.175

r = 0.200   r = 0.225   r = 0.250   r = 0.275

r = 0.300   r = 0.325   r = 0.350   r = 0.375

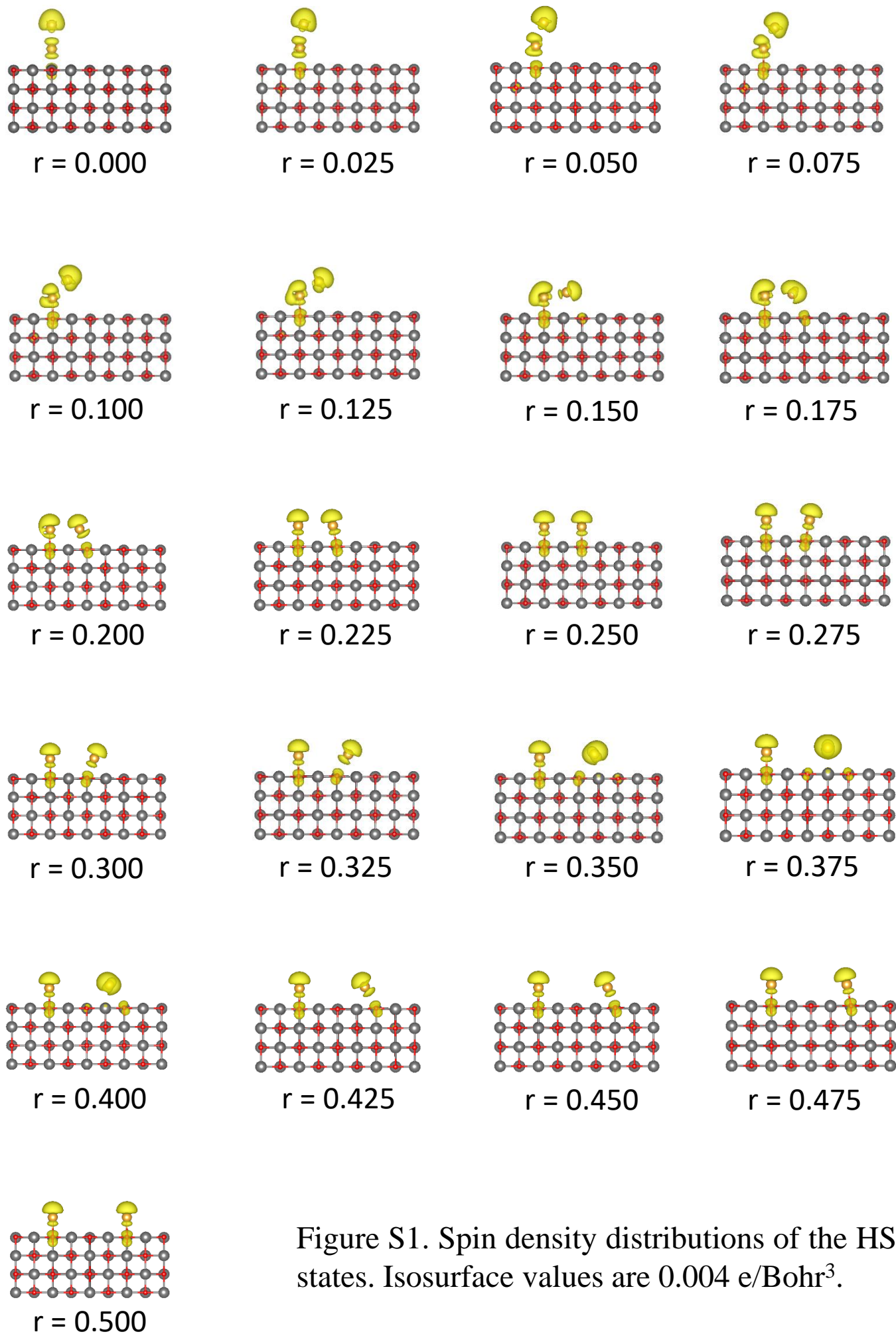r = 0.400   r = 0.425   r = 0.450   r = 0.475

r = 0.500

Figure S1. Spin density distributions of the HS states. Isosurface values are 0.004 e/Bohr^3.