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Adsorption and diffusion of hydrogen and oxygen in FCC-Co: a first-principles study

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Supporting Information

Table S1. Energy barrier E_a and diffusion prefactor D_0 of hydrogen and oxygen diffusion in Co and Ni derived from different computational methods and in comparison with available experimental data.

Diffusion Type	Method	Energy barrier (eV)	Diffusion prefactor (m^2/s)
H in Co	GGA (this work)	0.47	3.05×10^{-6}
	LDA (this work)	0.55	3.21×10^{-6}
	Exp. (Caskey et al. 1974)[a]	0.51	8.30×10^{-7}
H in Ni	*Ab initio* (Wimmer et al. 2008)[b]	0.47	3.84×10^{-6}
	Exp. (Völkl et al. 1978)[c]	0.42	6.90×10^{-7}
O in Co	GGA (this work)	1.03	1.29×10^{-6}
	LDA (this work)	1.17	1.34×10^{-6}
O in Ni	DFT-Phonon (Fang et al. 2014)[d]	0.92	8.00×10^{-6}
	Exp. (Zholobov et al. 1971)[e]	2.49	1.21×10^{-3}
	Exp.2 (Park et al. 1987)[f]	1.70	4.90×10^{-6}

[a]G. Caskey, R. Derrick and M. Louthan, *Scripta Metal*, 1974, **8**, 481-486.

[b]E. Wimmer, W. Wolf, J. Sticht, P. Saxe, C. B. Geller, R. Najafabadi and G. A. Young, *Phys Rev B*, 2008, **77**, 134305.

[c] J. Völkl and G. Alefeld, *Diffusion of hydrogen in metals*, Springer Berlin Heidelberg1978.

[d] H. Z. Fang, S. L. Shang, Y. Wang, Z. K. Liu, D. Alfonso, D. E. Alman, Y. K. Shin, C. Y. Zou, A. C. T. van Duin, Y. K. Lei and G. F. Wang, *J Appl Phys*, 2014, **115**, 043501.

[e] S. Zholobov and M. Malev, *Zh. Tekh. Fiz*, 1971, **41**, 677.

[f] J. W. Park and C. J. Altstetter, *Metallurgical Transactions A*, 1987, **18**, 43-50.