

The Adsorption Mechanism of Hydrogen on FeO Crystal Surfaces: A Density Functional Theory Study

Shujie Zhang ¹, Kejiang Li ^{1,*}, Yan Ma ², Yushan Bu ¹, Zeng Liang ¹, Zonghao Yang ¹
and Jianliang Zhang ¹

¹ School of Metallurgical and Ecological Engineering, University of Science and Technology
Beijing, Beijing 100083, China; shujiez@126.com (S.Z.); onion011213@163.com (Z.Y.)

² Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Dusseldorf, Germany

* Correspondence: likejiang@ustb.edu.cn

Table S1. Surface energy test results. The atoms that fix half the layers of the cell from the bottom up.

	total number of layers	Surface energy(J/m ²)
100	4	0.6835
	8	0.6854
	10	0.6871
110	6	1.3826
	8	1.4048
	12	1.4070
111-Fe	6	2.4044
	12	2.3993
111-O	6	1.3975
	12	1.3817