Electronic Supplementary Material

Influences of chosen force fields and applied load on thin film lubrication

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Table S1 Potential parameters of Buckingham potential for FeO and Fe_2O_3.

Atom	z (e)	B (eV)	ρ (Å)	C (Å^6 eV)
O	–0.945	9,022.821	0.265	85.092
Fe^{2+}	0.945	13,032.949	0.190	0.000
Fe^{3+}	1.4175	8,020.285	0.190	0.000

Note: Values for B, ρ, and C corresponding to iron cation–oxygen and oxygen–oxygen interaction, the cation–cation interaction being described only by Columbic repulsive forces.

$$r_{ij}^{o} = \left(\frac{(r_i^{o})^6 + (r_j^{o})^6}{2} \right)^{\frac{1}{6}} \tag{S1}$$

$$\varepsilon_{ij}^{o} = \frac{\sqrt[2]{\varepsilon_i^{o} \varepsilon_j^{o}} (r_i^{o} r_j^{o})^3}{(r_i^{o})^6 + (r_j^{o})^6} \tag{S2}$$

Table S2 Functional forms used in COMPASS FF. Reproduced with permission from Ref. [S1], © American Chemical Society 1998.

Potential name		Functional forms
Valence terms	Bond	$E_b = \sum_b [k_2(b-b_0)^2 + k_3(b-b_0)^3 + k_4(b-b_0)^4]$
	Angle	$E_\theta = \sum_\theta [k_2(\theta-\theta_0)^2 + k_3(\theta-\theta_0)^3 + k_4(\theta-\theta_0)^4]$
	Torsion	$E_\varphi = \sum_\phi [k_1(1-\cos\phi) + k_2(1-\cos 2\phi) + k_3(1-\cos 3\phi)]$
	Dihedral	$E_\chi = \sum_\chi k_2 \chi^2$
	Cross-coupling terms	$E_{cross} = \sum_{b,b'} k(b-b_0)(b'-b_0') + \sum_{b,\theta} k(b-b_0)(\theta-\theta_0) + \sum_{b,\phi} (b-b_0)[k_1\cos\phi + k_2\cos 2\phi + k_3\cos 3\phi]$ $+ \sum_{\theta,\phi} (\theta-\theta_0)[k_1\cos\phi + k_2\cos 2\phi + k_3\cos 3\phi] + \sum_{\theta,\theta'} k(\theta'-\theta_0')(\theta-\theta_0) + \sum_{\theta,\theta',\phi} k(\theta-\theta_0)(\theta'-\theta_0')\cos\phi$
Non-bond terms	Columbic interaction	$\sum_{i,j} \frac{q_i q_j}{r_{ij}}$
	van der Wall interaction	$\sum_{i,j} \epsilon_{ij} \left[2\left(\frac{r_{ij}^{o}}{r_{ij}}\right)^9 - 3\left(\frac{r_{ij}^{o}}{r_{ij}}\right)^6 \right]$

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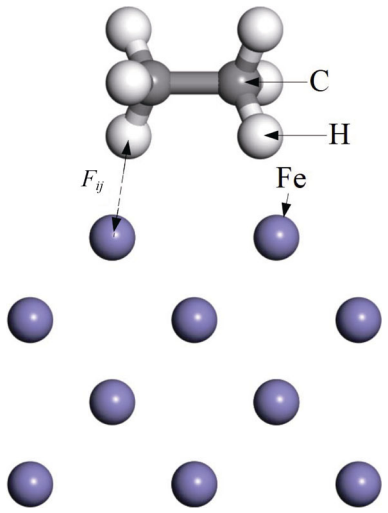

Fig. S1 Adsorption model of C_2H_6 adsorbate on Fe (100) surface reconstructed from reference [S2]. The interaction between ethane and iron surface was described using van der Wall interaction.

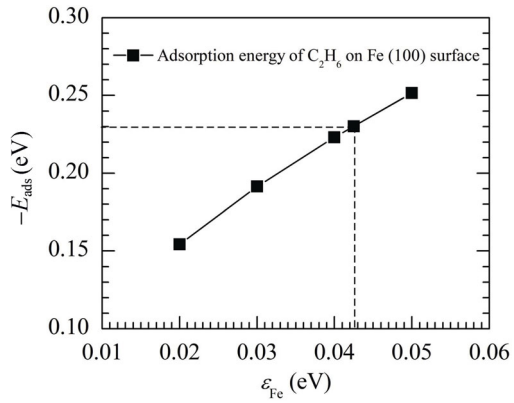

Fig. S2 Adsorption energy $-E_{ads}$ of ethane C_2H_6 on Fe (001) surface as a function of the well-depth energy of iron ε_{Fe}.

Table S3 Non-bond Lenard-Jones potential parameters for interaction between iron/iron oxide surfaces and hexadecane.

Atom	Zhao's work [S3]		Derived from COMPASS	
	ε_0 (eV)	r_0 (Å)	ε_0 (eV)	r_0 (Å)
O	0.0034	3.627	0.0097	3.627
Fe^{2+}	0.01858	3.950	—	3.950
Fe^{3+}	0.02149	4.077	—	4.077
Fe	ε_0 (eV)		r_0 (Å)	
	0.0425[a]		2.6595	

Table S4 Domain sizes of D_x, D_y, and D_z in x-, y-, and z-directions, respectively, as well as the number of hexadecane molecules for each confined shear model.

Surfaces	D_x (Å)	D_y (Å)	D_z (Å)	No. of $C_{16}H_{34}$ molecules
Fe	34.40	34.40	60.00	94
FeO	34.98	34.98	60.00	94
Fe_2O_3 (001)	34.88	35.25	60.00	94
Fe_2O_3 (012)	32.50	40.28	60.00	94

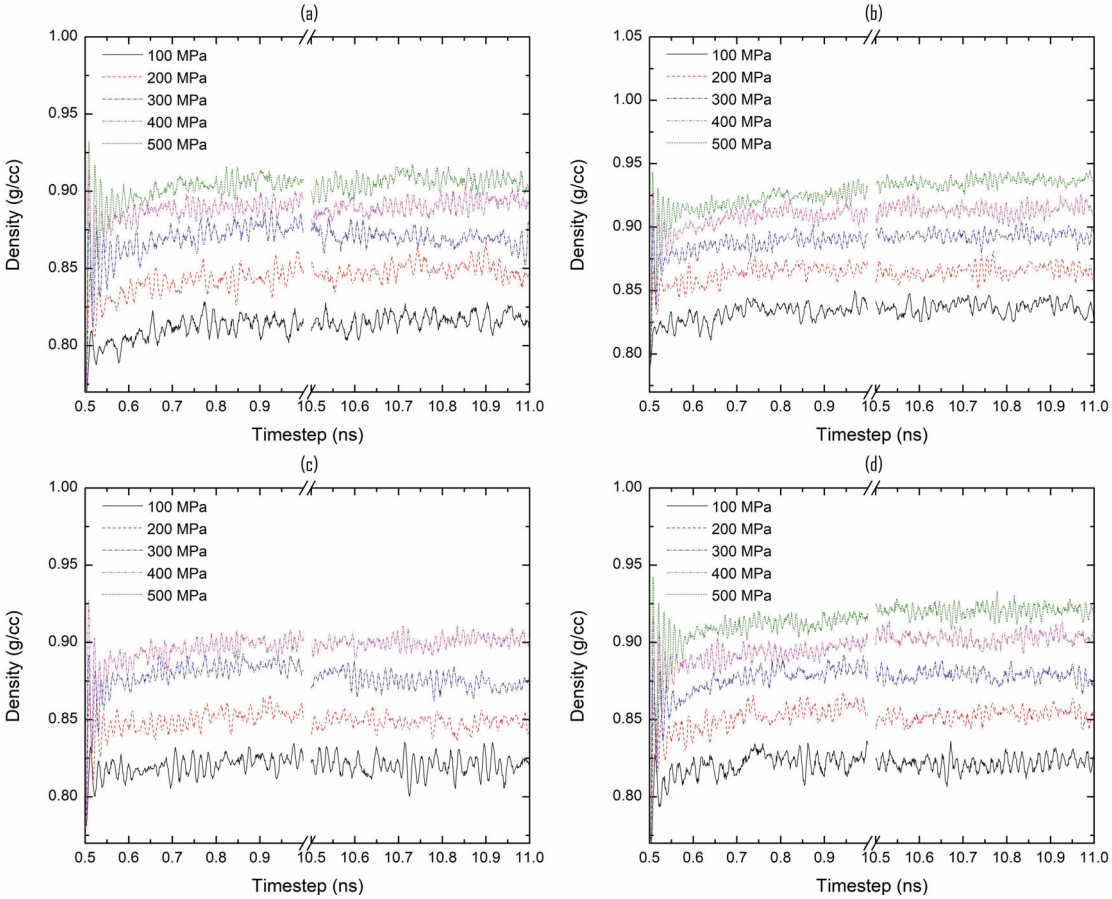

Fig. S3 Time evolution of hexadecane density at different applied loads for the cases of (a) Fe (100), (b) FeO (100), (c) Fe_2O_3 (0001), and (d) Fe_2O_3 (012) surfaces.

References

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