Supporting Information for ACS OMEGA

Spent coffee grounds as eco-friendly additives for aluminum-air batteries

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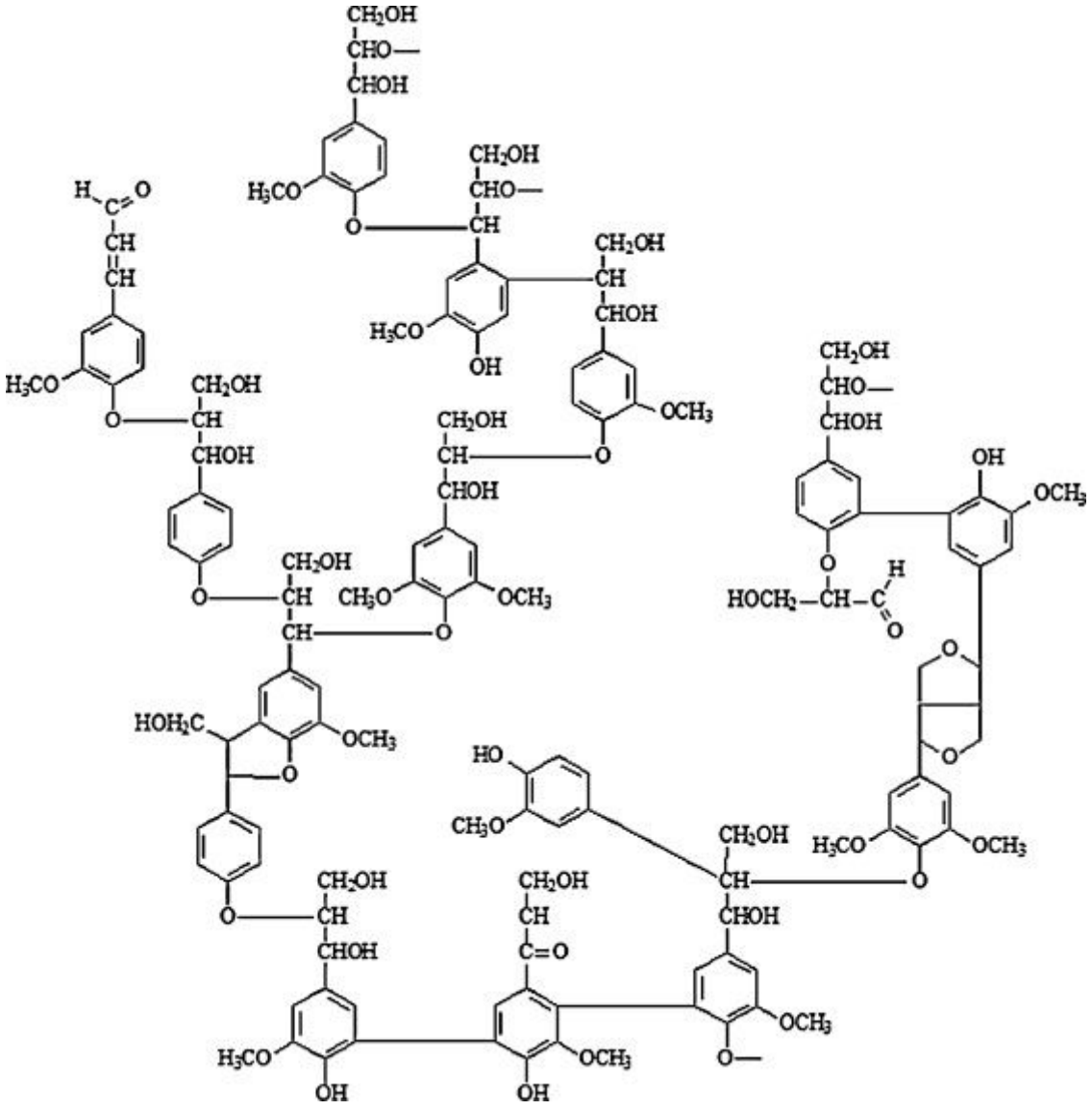


Figure S1. Representation of the lignin structure

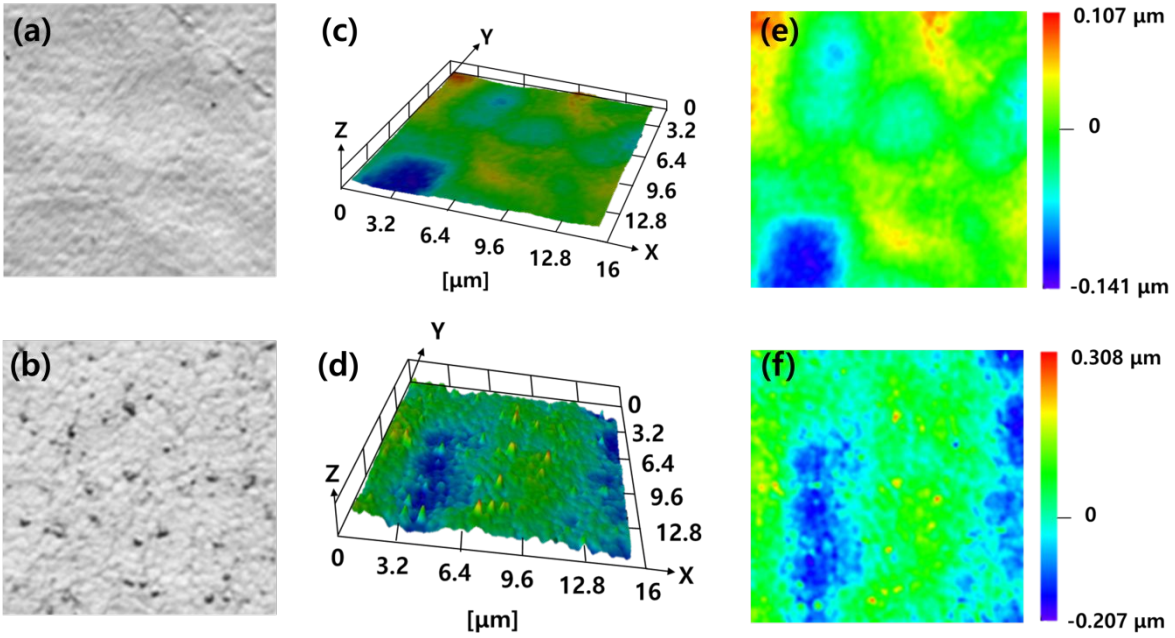


Figure S2. Laser scanning micrographs of aluminum surface after immersion in the absence of lignin molecules (a), (c), (e) and in the presence of lignin molecules (b), (d), (f): OM image of the surface without lignin molecules (a); 3D image of same area (c); 2D image of same area (e), OM image of the surface with lignin molecules (b); 3D image of same area (d); 2D image of same area (f).

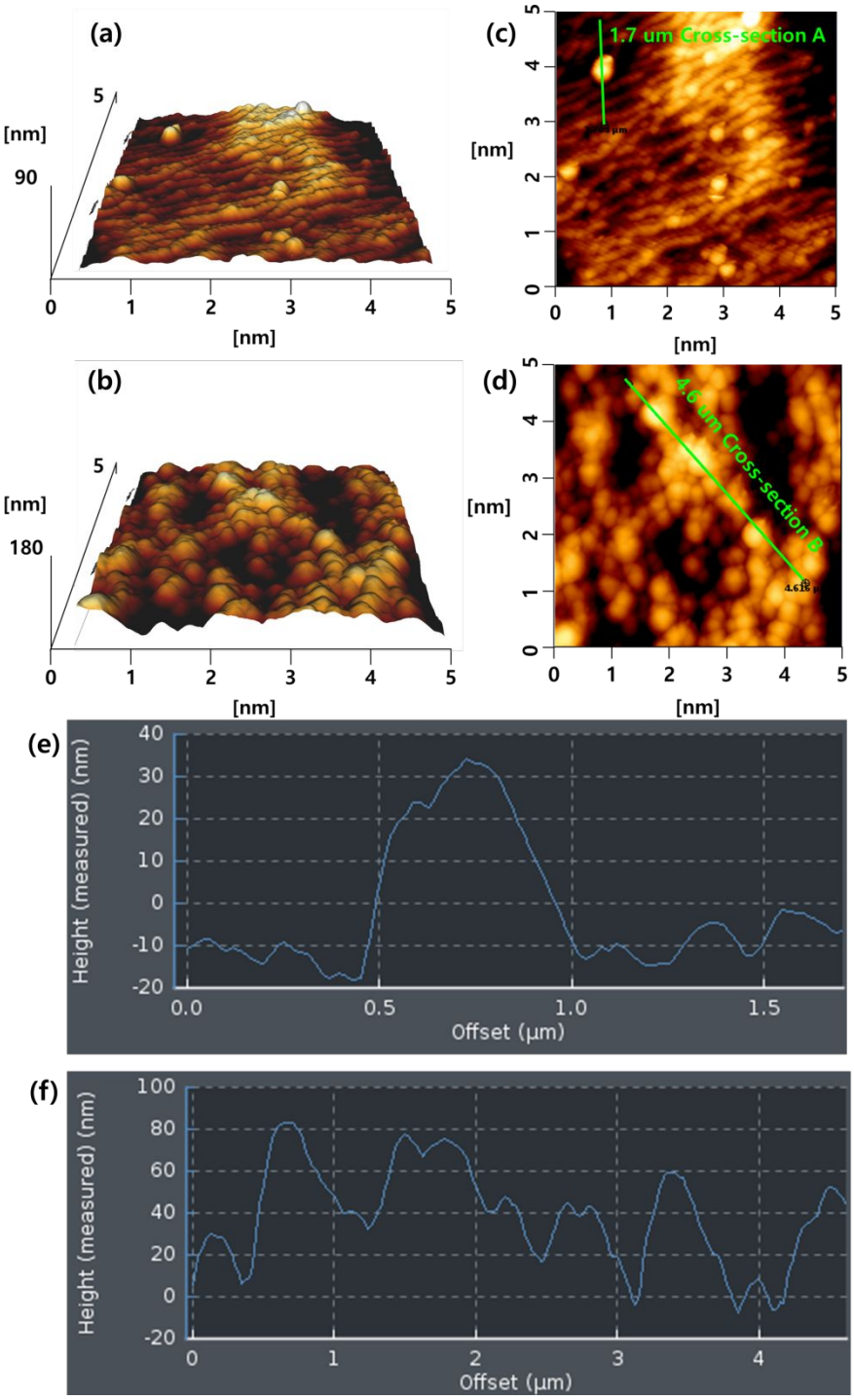


Figure S3. Atomic force micrographs of aluminum surface after immersion in the absence of lignin molecules (a), (c), (e) and in the presence of lignin molecules (b), (d), (f): 3D image of the surface without lignin molecules (a); 2D image of same area (c); Height profile on the

cross-section A (e), 3D image of the surface with lignin molecules (b); 3D image of same area (d); Height profile on the cross-section B (f).

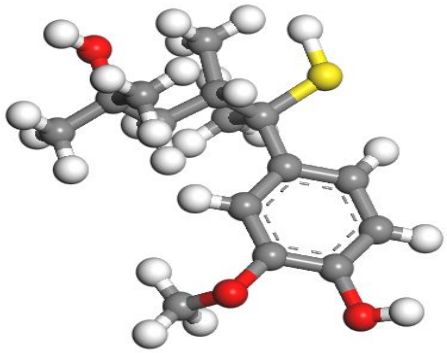
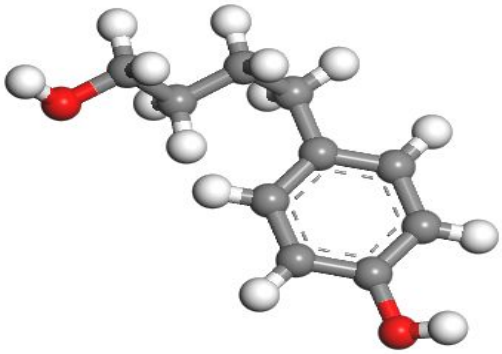
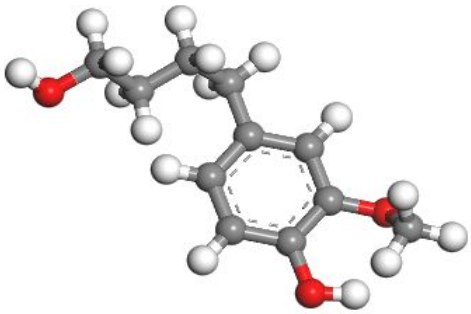
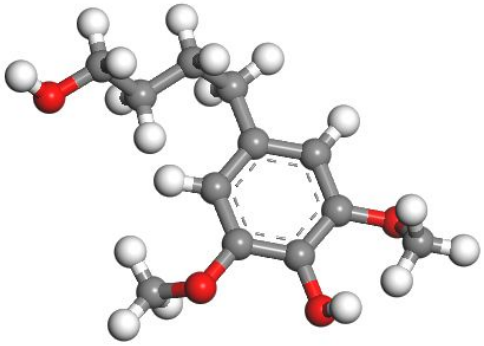
Isomer 1	Isomer 2
 -4182.3 eV	 -2490.7 eV
Isomer 3	Isomer 4
 -3119.4 eV	 -3748.3 eV

Figure S4. Optimized structures and relative energies for 4 types of geometrical conformers for lignin molecules

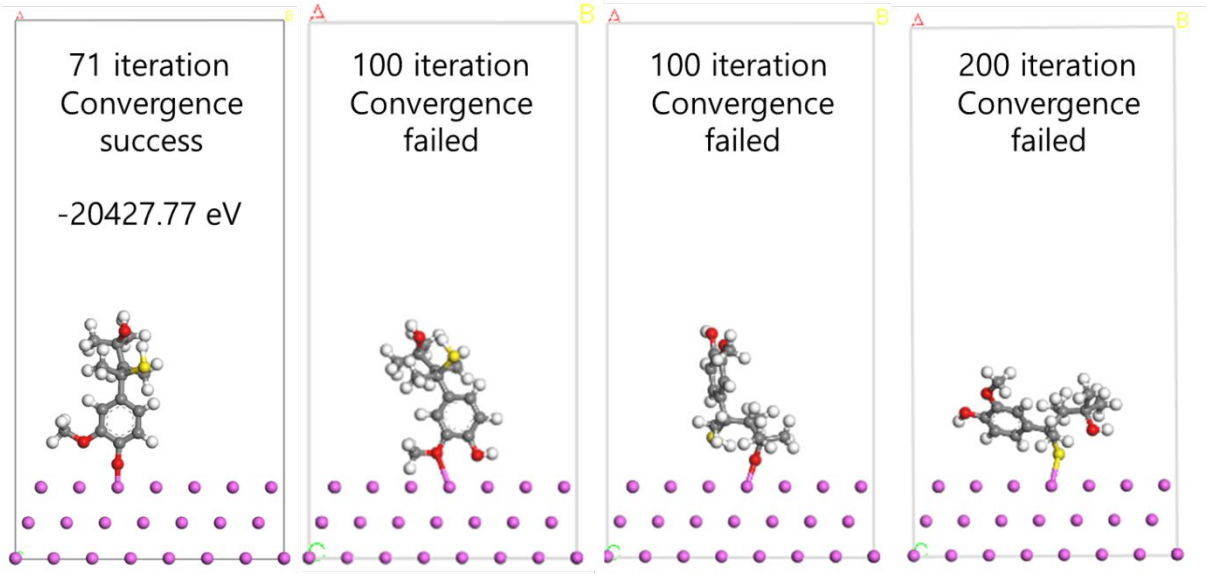


Figure S5. Geometrical optimization result for four different adsorption modes

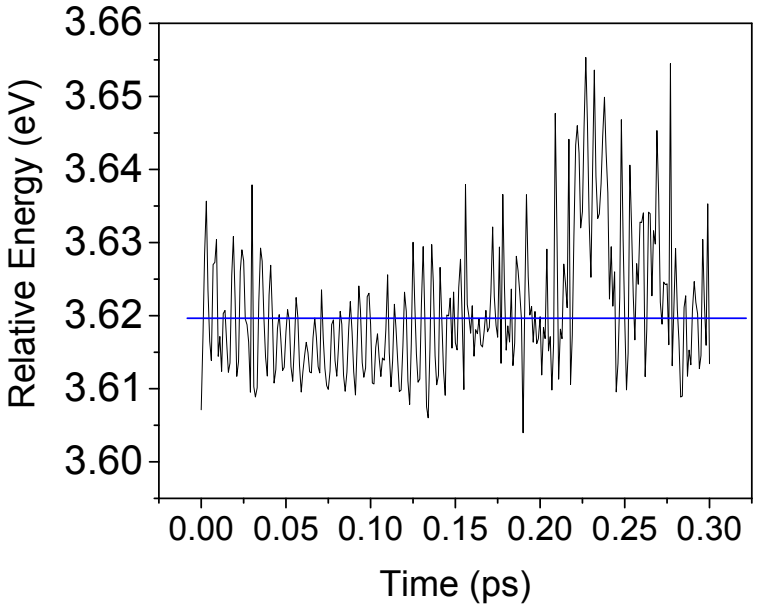


Figure S6. Total calculated energy variations (eV) during 0.3 ps of ab initio molecular dynamics (AIMD) simulation at 300k