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Electronic Supplementary Information

Interaction of Organic Compounds with Chondritic Silicate Surfaces. Atomistic Insights from Quantum Chemical Periodic Simulations

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Table S1. Contractions of the basis set employed in the work. Double-ζ* basis set were used to perform geometry optimizations and frequency calculations, triple-ζ* basis set for single point energy calculations to refine the adsorption energies.

Atom	double-ζ*	triple-ζ*
Si	(8s)–(831sp)–(1d)	(8s)–(6311sp)–(1d)
Mg	(8s)–(61sp)–(1d)	(8s)–(511sp)–(1d)
O (surface)	(6s)–(31sp)–(1d)	(8s)–(411sp)–(1d)
H	(31s)–(1p)	(311s)–(1p)
C	(6s)–(31sp)–(1d)	(511111s)–(411p)–(1d)
N	(6s)–(31sp)–(1d)	(511111s)–(411p)–(1d)
O (molecule)	(6s)–(31sp)–(1d)	(511111s)–(411p)–(1d)