Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supplementary Information

Spatial Arrangement of Dynamic Surface Species from Solid-State NMR and Machine Learning-Accelerated MD Simulations

Takeshi Kobayashi,[a*] Da-Jiang Liu[a*] and Frédéric A. Perras[a]

[a] U.S. DOE Ames National Laboratory, Ames, IA, 50011, USA

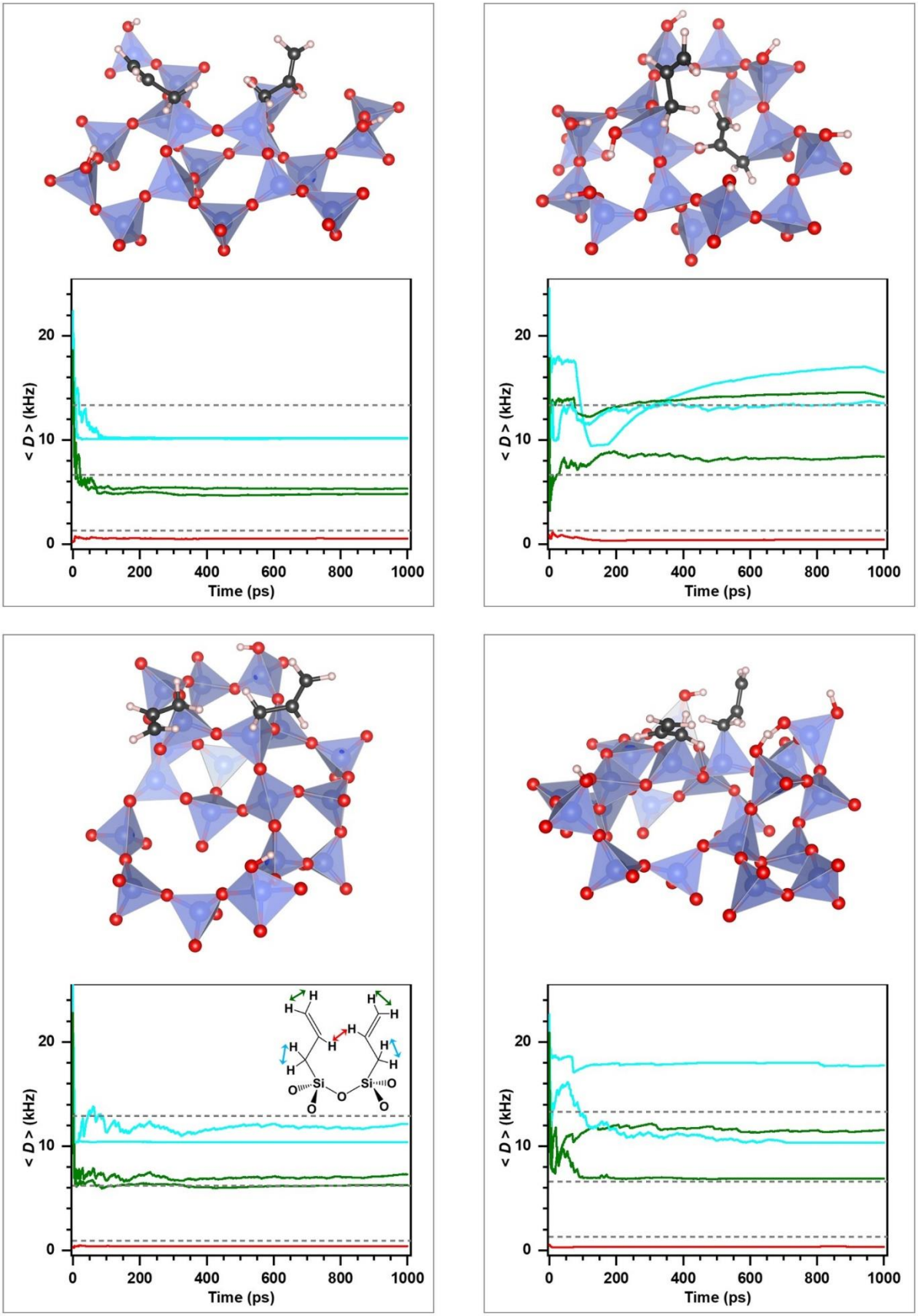

Fig. S1 Arrangement of AL groups on the silica surface and the evolution of $^{1}H–^{1}H$ dipolar coupling constants as a function of the DeePMD simulation time. Purple tetrahedra represents SiO_4. Red, white, and grey spheres represent oxygen, hydrogen, and carbon atoms, respectively. Not all atoms used for the MD simulations are shown for visual clarity.

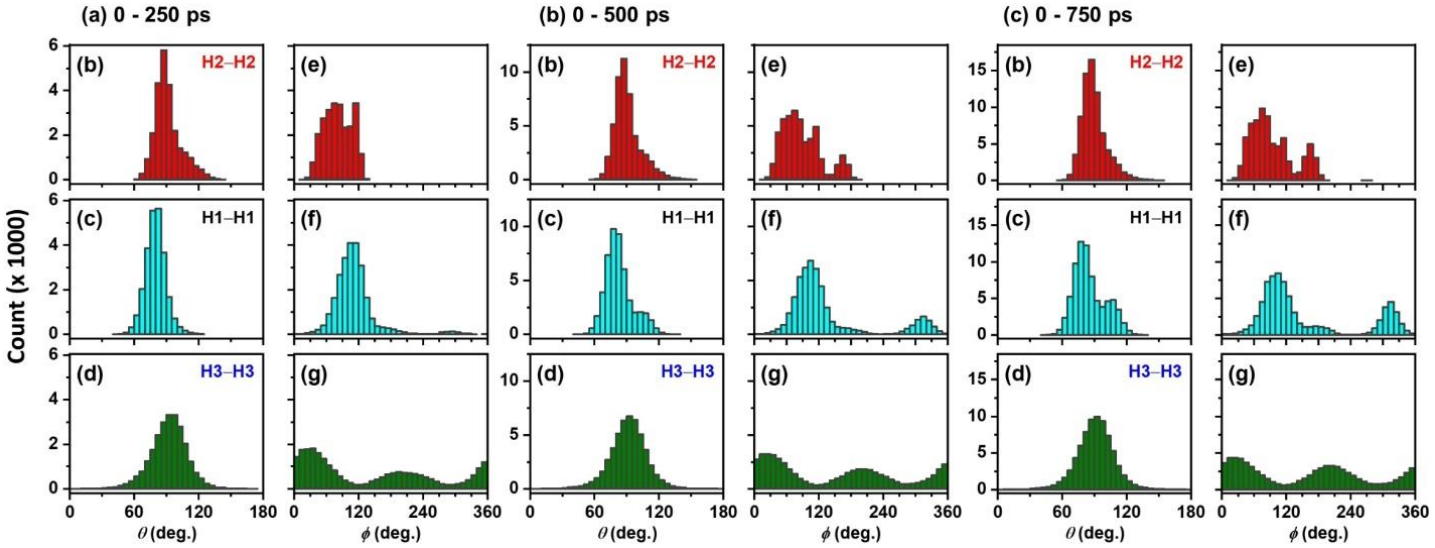

Fig. S2 Histograms of θ and ϕ between 0 s and 250 ps (a), 0 s and 500 ps (b), and 0 s and 750 ps (c) from the DeePMD simulation of the model shown in Fig. 3a.

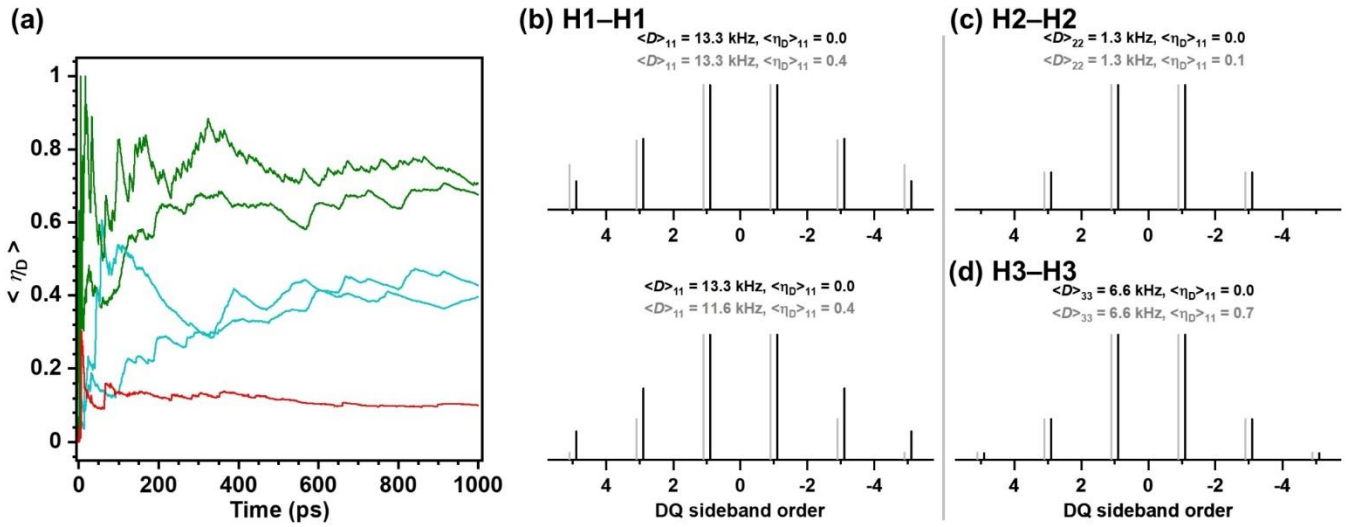

Fig. S3 (a) The evolution of asymmetry parameter of ^{1}H–^{1}H dipolar coupling for the model shown in Fig. 3a as a function of the DeePMD simulation time. (b-d) Simulations comparing the DQ sideband manifolds obtained with and without the inclusion of η_D.

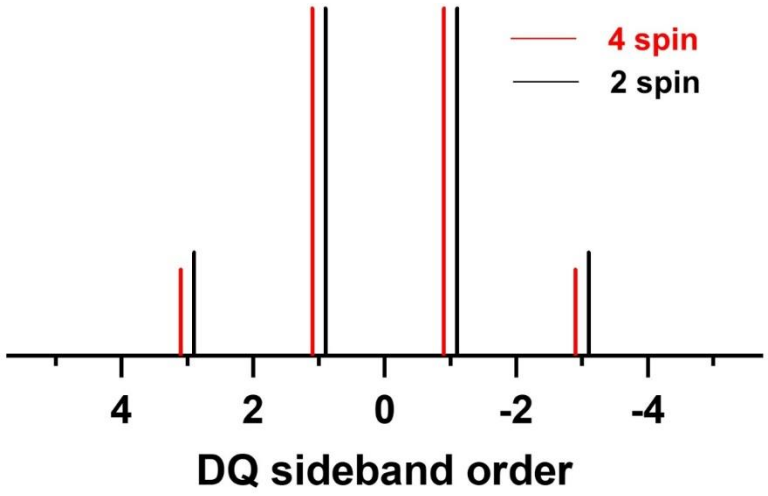

Fig. S4 Comparison of H2–H2 DQ sideband patterns simulated with 2 and 4 spin systems. The 4 spin simulation involves additional two H1 protons as –C(–H1)$_2$–C(–H2)= and –C(–H2)=, where the H1–H1($\langle D \rangle_{11}$ = 11.6 kHz) and H1–H2 ($\langle D \rangle_{12}$ = 2 kHz) intramolecular dipolar couplings are taken into account.

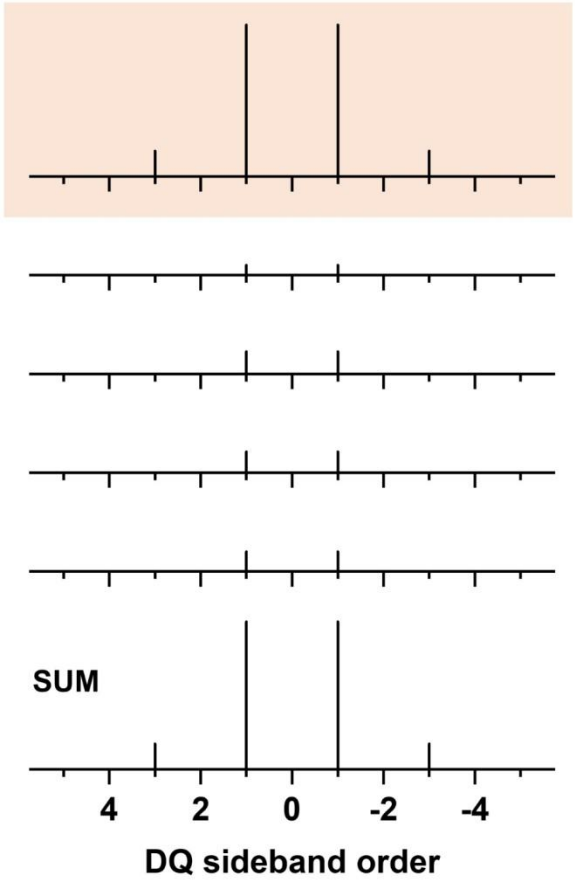

Fig. S5 Simulated H2–H2 DQ sideband patters for all models and their sum (bottom). The model shown in Fig. 3a showed much more intense DQ-filtered signals as compared to other models and is the only model that yields observable sidebands at ±3. Given that, Fig. 3a is considered a representative model of the localized functional groups.