Supplemental Material For:

Hybridization of Surface Waves with Organic Adlayer Librations: A Helium Atom Scattering and Density Functional Perturbation Theory Study of Methyl-Si(111)

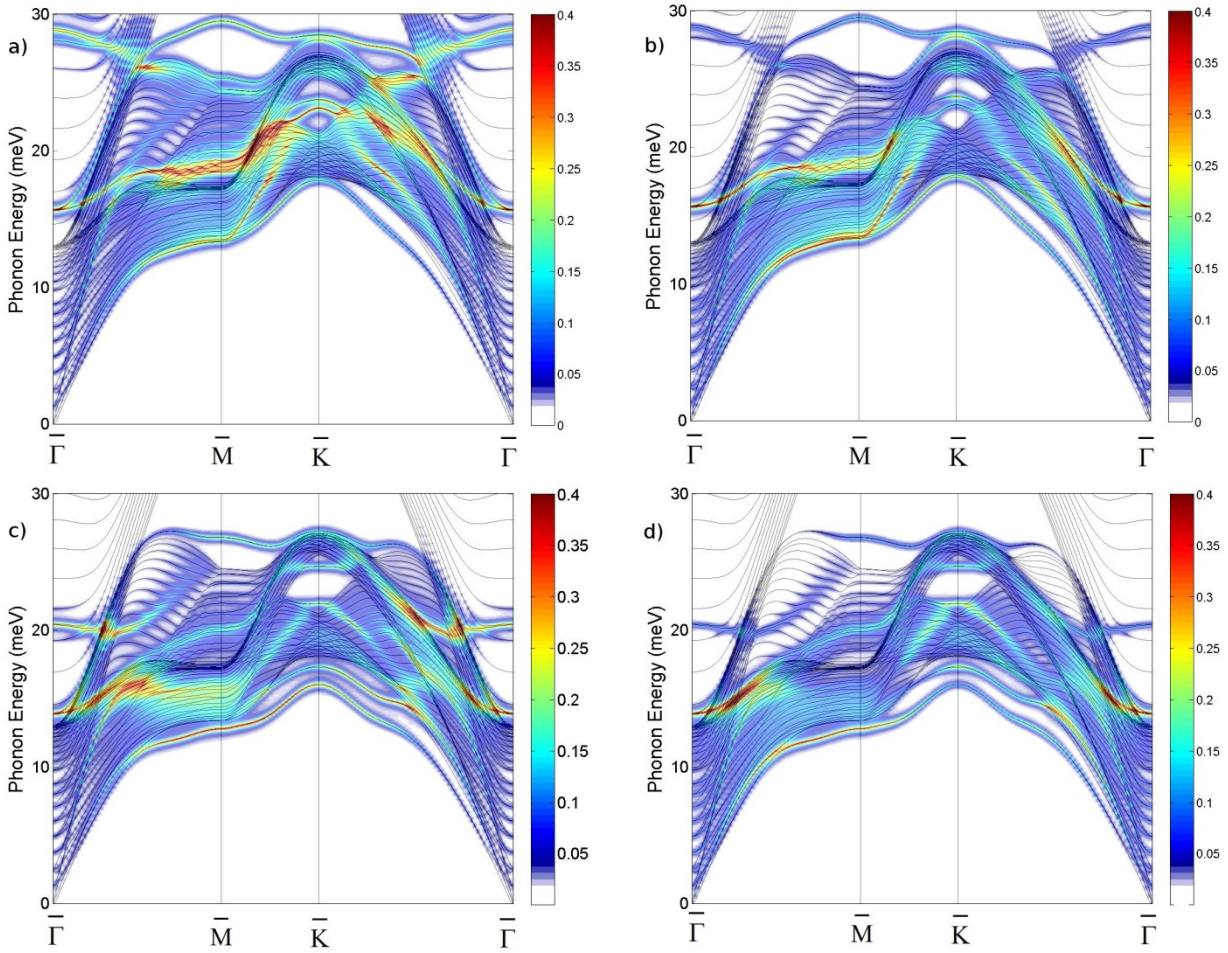
Ryan D. Brown, Zachary M. Hund, Davide Campi, Leslie E. O'Leary, Nathan S. Lewis, M. Bernasconi, G. Benedek, and S. J. Sibener[‡]
[‡]Corresponding author; Email s-sibener@uchicago.edu

Figure Captions

FIG. S1.

Phonon density of states for modes with in-plane polarization for Si-CH_3 projected onto the H atoms (a), the C atom (b) and for Si-CD_3 projected onto D atoms (c) and the C atom (d), with intensity given by the color scale. The comparison between (a) and (c) highlights the different energies of the hindered rotations due to the isotopic substitution. Hindered rotations, characterized by a large projection on H or D and by a minor projection on C, go from 29 meV at $\bar{\Gamma}$ to 24 meV at $\bar{K}$ for CH_3-Si(111) and from 21 meV at $\bar{\Gamma}$ to 16 meV at $\bar{K}$ for CD_3-Si(111) . Rocking modes (which exhibit a large projection both on H, or D, and C) are slightly affected by the isotopic effect and have an energy of approximately 15 meV both for surfaces at $\bar{\Gamma}$, and hybridize in similar way with Rayleigh wave near the zone edge.

FIG. S1.


a)
b)
c)
d)
Phonon Energy (meV)
30
20
10
0
Γ̄
M̄
K̄
Γ̄
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0