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End Functional Hydrogen Bonding Modulates Odd-Even Effect in Alkanethiol Monolayer Assembly[1] KSHITIJ JHA, YENENEH YIMER, MESFIN TSIGE, The University of Akron — Hydroxyl (-OH) terminated n-alkanethiols on gold show a two-dimensional zig-zag nature for the top hydrogen bonded network. We observe transfer of packing characteristics from top network to the buried ad-atom (sulfur) distribution quantified as occupancy percentages for atop, hollow (fcc and hcp), and bridge sites. Employing validated metal potentials and all-atom molecular dynamics, we also quantify the dynamic correlation between the top layer (end-functional) and ad-layer (thiol) through variance in distribution peaks for nearest neighbors as a function of temperature. The hydrogen bond network and packing of the monolayer increases in strength with chain length for OH terminated n-alkanethiols. Shorter chain lengths lead to better transfer of packing, for a given network strength. Odd chain lengths, compared to even, have a lower lattice spacing by an average of 0.04 Å. The transfer effect of the top network is not observed, as expected, for methyl (-CH_3) terminated n-alkanethiols since there is no hydrogen bonding. Trends in packing and transfer for monolayer assembly could provide design principles for polymer based nanoactuators and sensors.

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