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A low friction coefficient between graphane coated surfaces CAN ATACA, Department of Physics, Bilkent University, Ankara, Turkey, 06800, HASAN SAHIN, UNAM-Material Science and Nanotechnology, Bilkent University, Ankara, Turkey, 06800, SALIM CIRACI, Department of Physics, Bilkent University, Ankara, Turkey, 06800; UNAM-Material Science and Nanotechnology, Bilkent University, Ankara, Turkey, 06800 — Using first-principles calculations, we investigate the electronic properties and stability of recently synthesized 2D hydrocarbon in honeycomb structure, namely graphane. Varios charge analysis result that in graphane geometry negatively charged carbon atoms are sandwiched between positively charged hydrogen atoms bound from both sites. In addition high frequency vibration modes associated with C-H bonds are well separated from the rest of the spectrum. The repulsive interaction between two graphane layers due to mainly strong Coulomb interaction serves as if a boundary lubricant and prevents the sliding graphane surfaces from being closer to each other even under high normal forces. As a result, calculated lateral force variation generated during sliding has small magnitude under high constant loading forces. Superlow friction observed earlier between diamond-like carbon-coated surfaces can be understood strong and stiff carbon-carbon and carbon-hydrogen bonds which do not favor energy dissipation.

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