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Development of accurate potentials to explore the structure of water on 2D materials. KARTEEK BEJAGAM, Virginia Tech , SAMRENDRA SINGH, Scientist, SANKET DESHMUKH, Assistant Professor, DESHMKUH GROUP TEAM, SAMRENDRA GROUP COLLABORATION — Water play an important role in many biological and non-biological process. Thus structure of water at various interfaces and under confinement has always been the topic of immense interest. 2-D materials have shown great potential in surface coating applications and nanofluidic devices. However, the exact atomic level understanding of the wettability of single layer of these 2-D materials is still lacking mainly due to lack of experimental techniques and computational methodologies including accurate force-field potentials and algorithms to measure the contact angle of water. In the present study, we have developed a new algorithm to measure the accurate contact angle between water and 2-D materials. The algorithm is based on fitting the best sphere to the shape of the droplet. This novel spherical fitting method accounts for every individual molecule of the droplet, rather than those at the surface only. We employ this method of contact angle measurements to develop the accurate non-bonded potentials between water and 2-D materials including graphene and boron nitride (BN) to reproduce the experimentally observed contact angle of water on these 2-D materials. Different water models such as SPC, SPC/Fw, and TIP3P were used to study the structure of water at the interfaces.

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