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SuAVE: Surface Assessment via Grid Evaluation for Every Surface Curvature and Every Cavity Shape

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Abstract: The Surface Assessment via Grid Evaluation (SuAVE) software was developed to account for the effect of curvature in the calculations of structural properties of chemical interfaces regardless of chemical composition, asymmetry, and level of atom coarseness. It employs differential geometry techniques, enabling the representation of chemical surfaces as fully differentiable. In this article, we present novel developments of SuAVE to treat closed surfaces and complex cavity shapes. These developments expand the repertoire of curvature-dependent analyses already available in the previous version of SuAVE (*e.g.* area per lipid, density profiles, membrane thickness, deuterium order parameters, volume per lipid, surface curvature angle) to include new functionalities applicable to soft matter (*e.g.* sphericity, average radius, principal moment of inertia and roundness) and crystalline porous materials (*e.g.* pore diameter, internal void volume, total area, and the total void volume of the unit cell structure). SuAVE can accurately handle chemical systems with high and low atom density as demonstrated for two distinct chemical systems: the Lipid-A vesicle and a set of selected metal organic frameworks (MOFs). The SuAVE software v2.0 is fully parallel and benefits from a compiler that supports OpenMP. SuAVE is freely available from https://github.com/SuAVE-Software/source and https://www.biomatsite.net/.

Key-words: Phase Transitions, Soft-Matter, Crystalline Materials, Complex Shapes

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References:

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