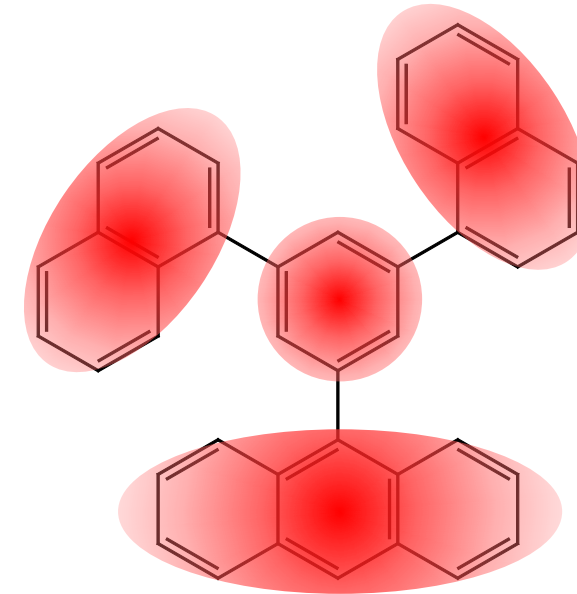


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Atomistic simulations are a powerful technique for materials science, but needing to track the motion of every single atom makes simulations of complicated materials for long times prohibitively difficult. Coarse-graining is one way around this problem. Coarse-graining groups atoms together into spherical beads, then only tracks the beads, reducing computational cost. This simplification enables simulations of slow processes and complex systems.

Wisconsin MRSEC researchers have developed a coarse-graining technique called AniSOAP (for anisotropic smooth overlap of atomic potentials) that gives the beads shapes that reflect the shape of the molecules they represent. This simple idea – carefully implemented to be mathematically rigorous and account for how molecules typically interact – can be used for high-accuracy coarse grained simulations or to understand materials behavior that depends on molecular shape or orientation. AniSOAP is also particularly useful for machine learning analysis of molecular behavior using simple, physically-interpretable algorithms, producing new insight for researchers.



Wisconsin MRSEC Researchers created new anisotropic machine learning descriptor for molecular materials called AniSOAP, which incorporates information about molecule shape. This figure demonstrates how a triarylbenzene molecule is represented by AniSOAP as a set of ellipses, each of which covers several atoms.