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Real-Time Molecular Visualization Supporting Diffuse Illumination and Ambient Occlusion

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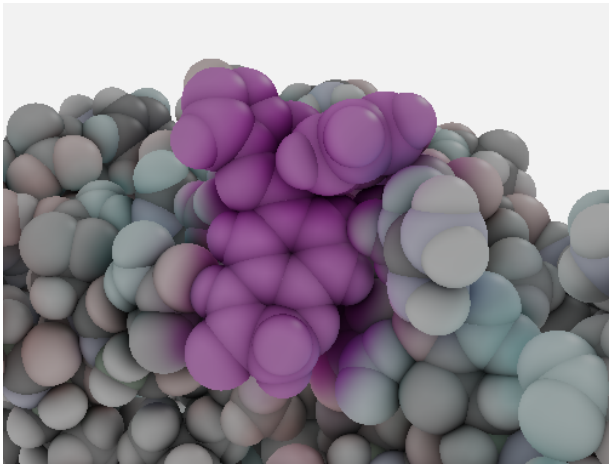

Today molecular simulations produce complex data sets capturing the interactions of molecules in detail. Due to the complexity of this time-varying data, advanced visualization techniques are required to support its visual analysis. Current molecular visualization techniques utilize ambient occlusion as a global illumination approximation to improve spatial comprehension. Besides these shadow-like effects, interreflections are also known to improve the spatial comprehension of complex geometric structures. Unfortunately, the inherent computational complexity of interreflections would forbid interactive exploration, which is mandatory in many scenarios dealing with static and time-varying data. In this paper, we introduce a novel analytic approach for capturing interreflections of molecular structures in real-time. By exploiting the knowledge of the underlying space filling representations, we are able to reduce the required parameters and can thus apply symbolic regression to obtain an analytic expression for interreflections. We show how to obtain the data required for the symbolic regression analysis, and how to exploit our analytic solution to enhance interactive molecular visualizations.

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