

Supplementary material: A General Illumination Model for Molecular Visualization

P. Hermosilla¹, P. Vázquez², A. Vinacua², T. Ropinski¹

¹Visual Computing Group, Ulm University, Ulm, Germany
²VIRVIG Group, Universitat Politècnica de Catalunya, Barcelona, Spain

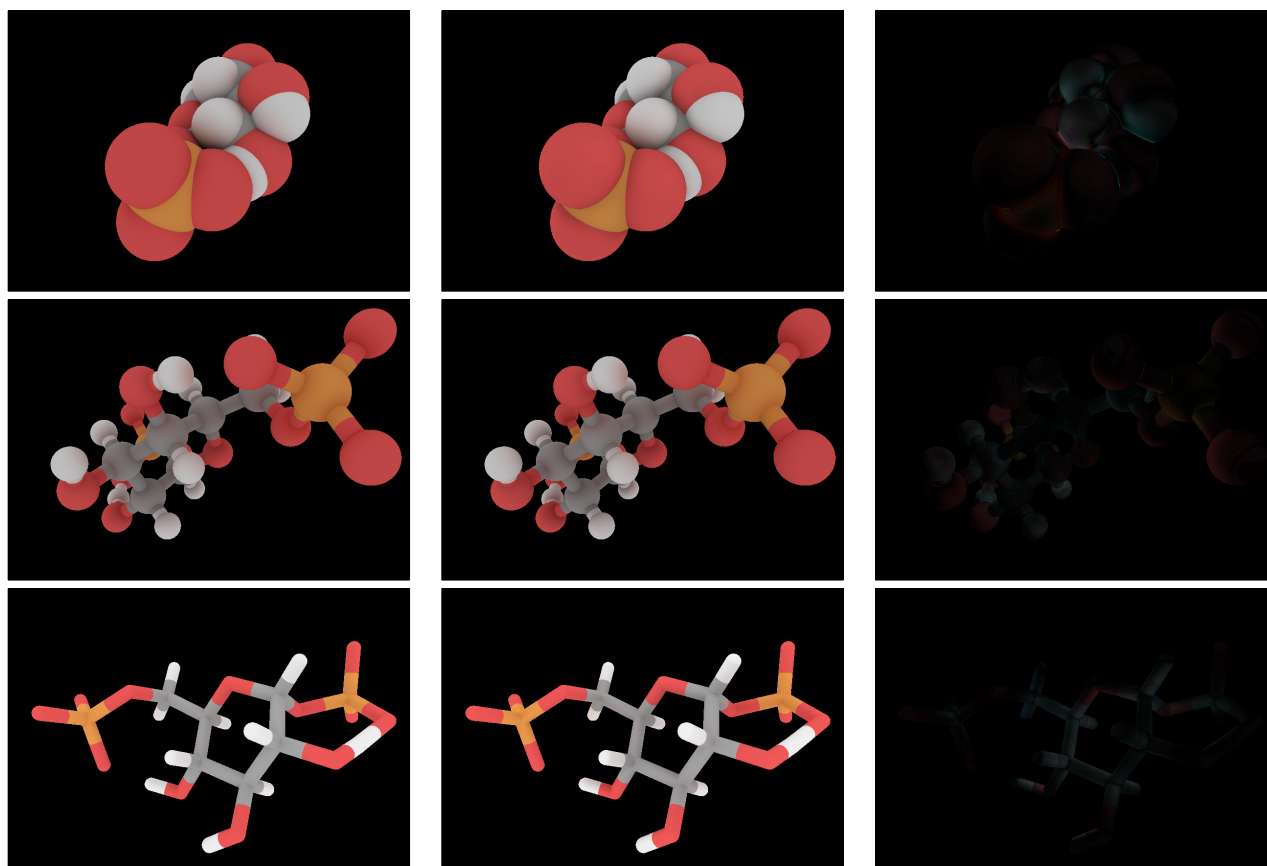


Figure 1: We compared our illumination model (right images) with the results of a path-tracing algorithm (middle images). Whilst the Balls-and-Sticks and Licorice models achieve very similar results, the Space-filling model generates less pronounced shadows, though still plausible. And the diffuse interactions appear in the same areas as with the path tracing algorithm. Moreover, we provide images of the (amplified) differences between the images generated by our algorithm and the images generated by the path-tracing algorithm.

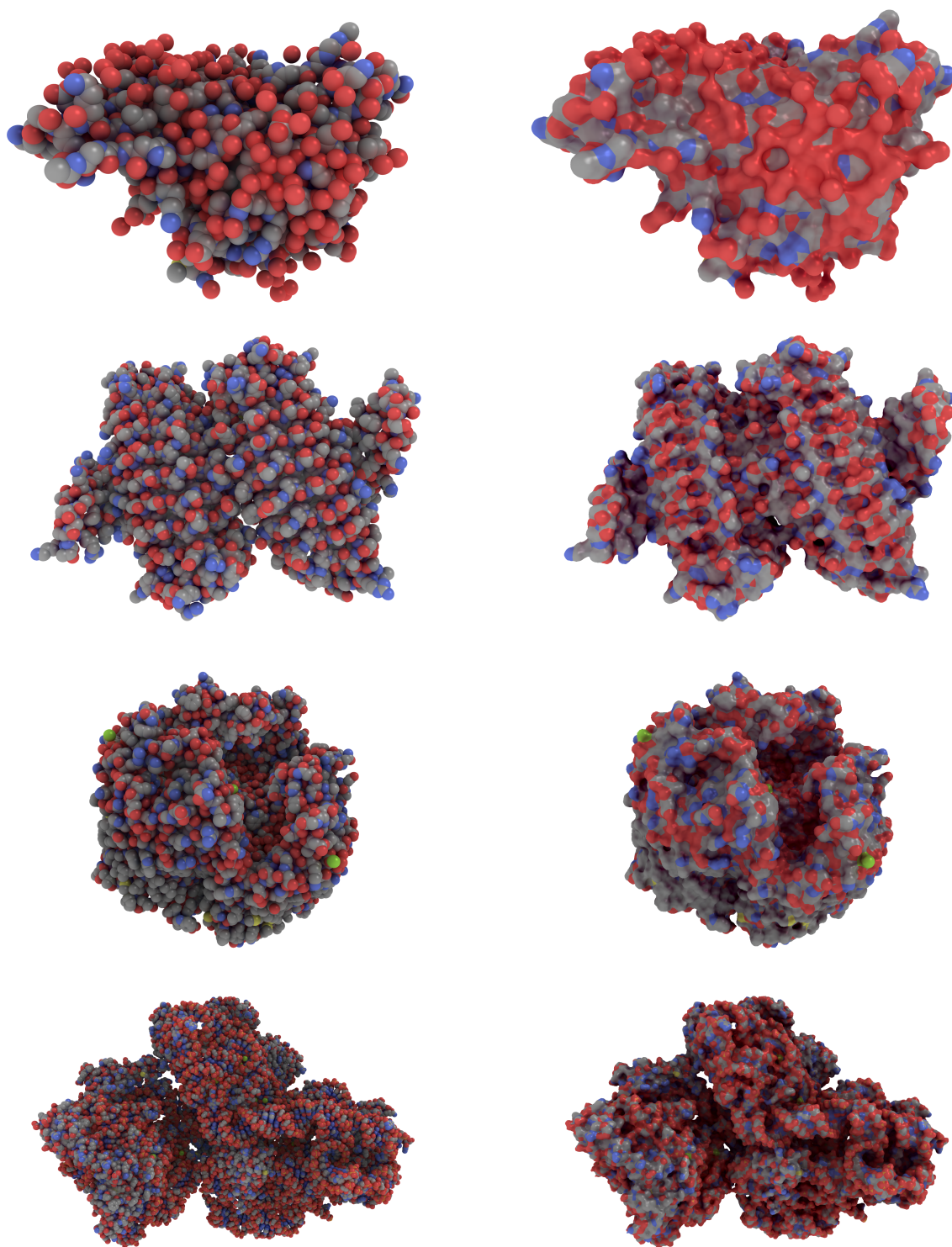


Figure 2: Figures of the molecules used to measure the performance of our method (Table 1 of the paper) represented by the Space-filling model (left) and by their Solvent Excluded Surfaces (right): 1OGZ (first row), 4NKG (second row), IAF6 (third row), and 5XYU (last row).

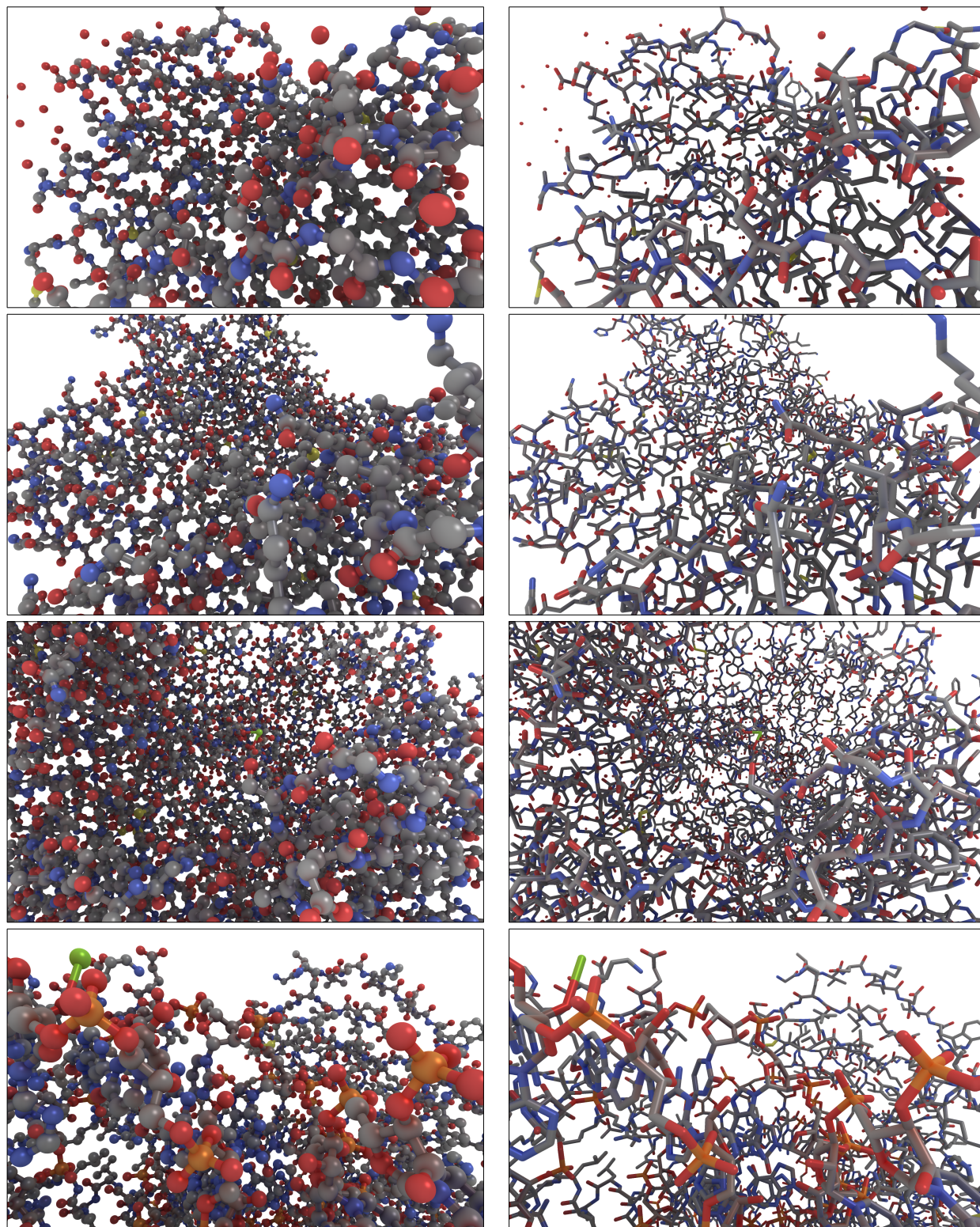


Figure 3: Figures of the molecules used to measure the performance of our method (Table 1 of the paper) represented by the Balls-and-Sticks (left) and the Licorice (right) models: 1OGZ (first row), 4NKG (second row), 1AF6 (third row), and 5XYU (last row).