Features	PyRID	ReaDDy	MCell	Smoldyn
Reactions	🟢 Very Good (zeroth order, unimolecular, bimolecular, arbitrary number of products, compartment specific, different reaction paths)	🟢 Very Good (not compartment specific however!)	🟢 Excellent (Integration with BioNetGen)	🟢 Excellent (Integration with BioNetGen)
Reaction accuracy	🟡 Volume: Good (Not exact close to boundary, reversible fusion reactions of interacting particles do not obey detailed balance) 🟡 Surface: Good (euclidian distance only)	🟢 Volume: Very Good (Not exact close to boundary, reversible fusion reactions obey detailed balance) 🟡 Surface: Good (euclidian distance only)	🟢 Volume: Very Good, 🟢 Surface: Very Good	🟢 Volume: Very Good, 🟢 Surface: Very Good
Diffusion	🟢 Anisotropic translational and rotaional diffusion, integrated diffusion tensors calculation	🟡 Isotropic translational diffusion	🟡 Isotropic translational diffusion	🟡 Anisotropic translational diffusion
Molecular structure	🟢 Molecules modeled explicitly (by interaction potential and /or rigid bodies).	🟡 Molecules modeled explicitly (only by interaction potential).	🔴 Indirectly by internal state variables (only point particles).	🔴 Indirectly by internal state variables (spherical particle approximation).
Surfaces	🟢 Arbitrary surfaces (triangulated mesh, supports obj. format)	🟡 Only via external potentials (Box and Sphere)	🟢 Arbitrary surfaces triangulated mesh, blender interface)	🟢 Arbitrary surfaces (6 elementary shapes, custom format)
Interactions	🟢 Selection of several pair-potentials, custom potentials can be added easily.	🟢 Selection of 4 potentials, custom potentials require altering C++ source code.	🔴 No Interactions	🔴/🟡 Excluded volume approximation for spheres.
Boundary Conditions	🟢 Periodic, Repulsive, Fixed concentration	🟡 Periodic, Repulsive	🟢 Periodic, Repulsive, Fixed concentration	🟢 Periodic, Repulsive, Fixed concentration
Polydispersity	🟢 Efficient simulation of polydisperse system by the use of a hierarchical grid data structure	🟡 Polydisperse systems result in performance drop.	Does not apply	Does not apply
API	🟢 Python	🟢 Python	🟢 Blender GUI, Python	🟢 Python, Text based
Modifiability	🟢 Excellent (All source code in python, little dependencies)	🟡 Ok (Requires changing C++ source code)	🟡 Ok (Requires changing C++ source code)	🟡 Ok (Requires changing C++ source code, Libsmoldyn API)