Minimum Chips

Parallel algorithms for the structures of fluids

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How many chips is the minimum?

Figure 1: Some chips

Minimum chips implements mathematical operations on a large array for use with high performance computing systems. The array is split into blocks, each one of which is shared between one or more MPI processes. The code is optionally accelerated with OpenMP pragmas.

Both Monte-Carlo simulations of material properties, and solvers for integral equations for the structures of fluids have been built on the foundation implemented in `minimum_chips`.

The most expensive step in the solution of integral equations for the structures of fluids of particles with internal structure is ideal for GPGPU acceleration. CUDA is used for this step.
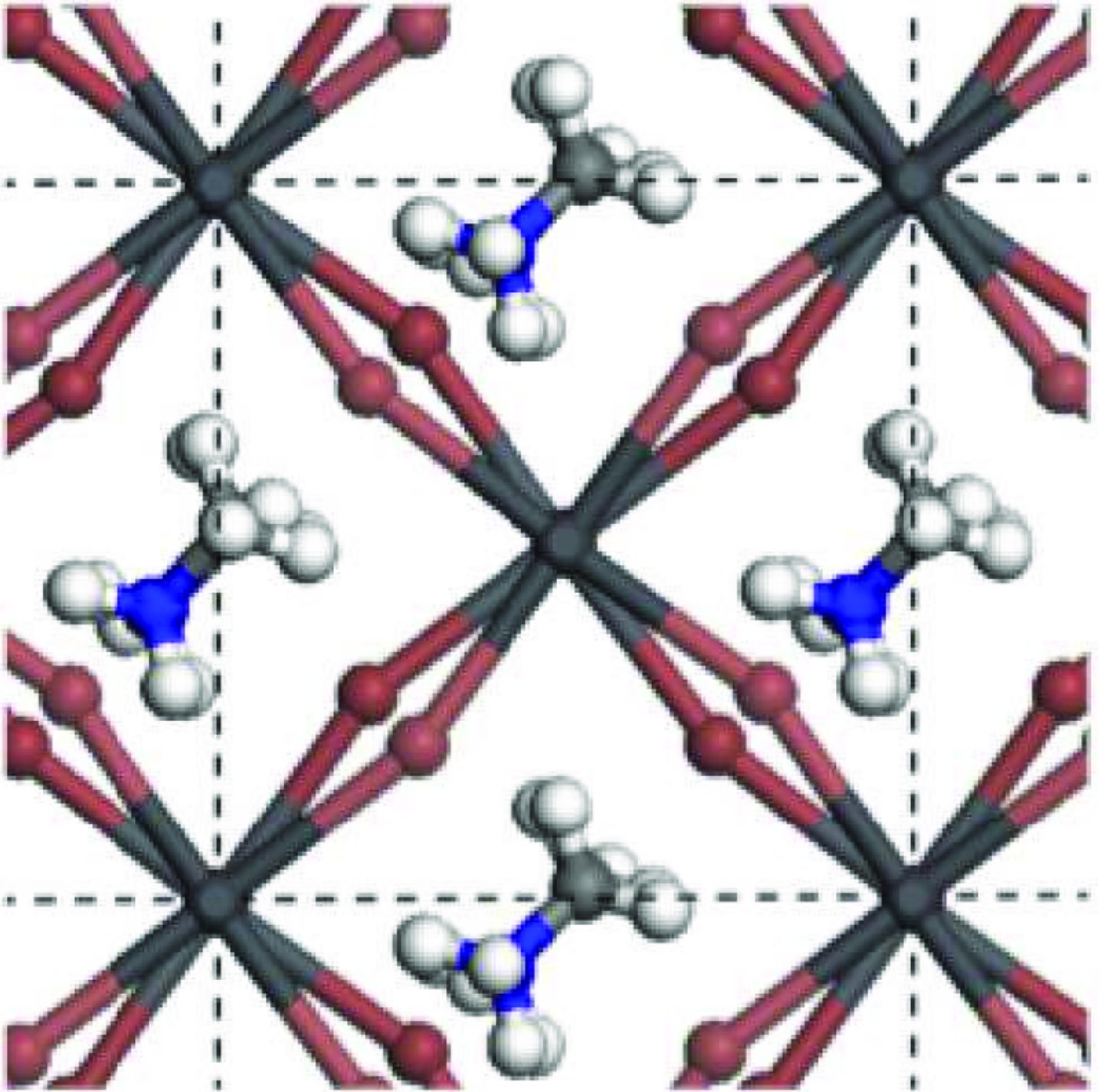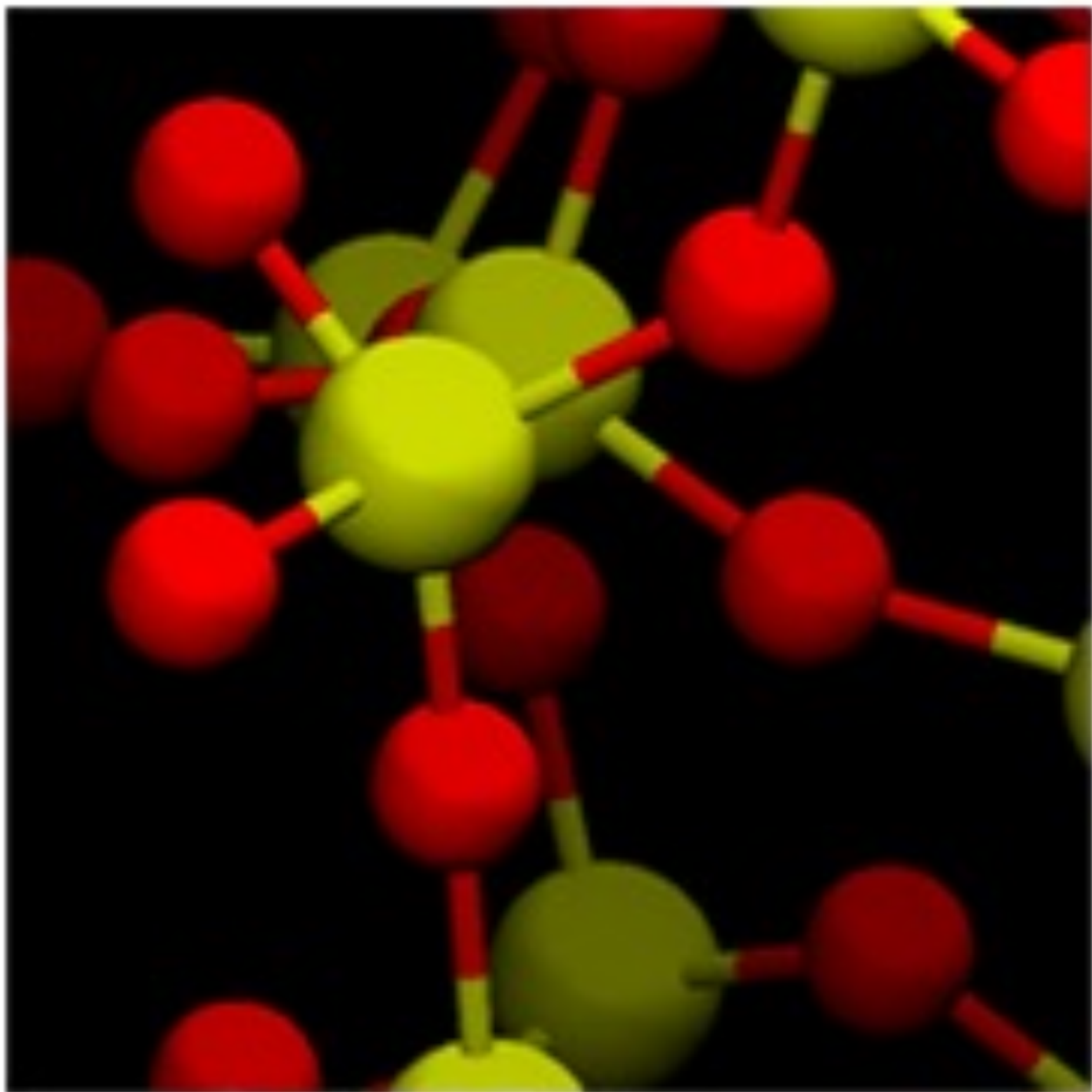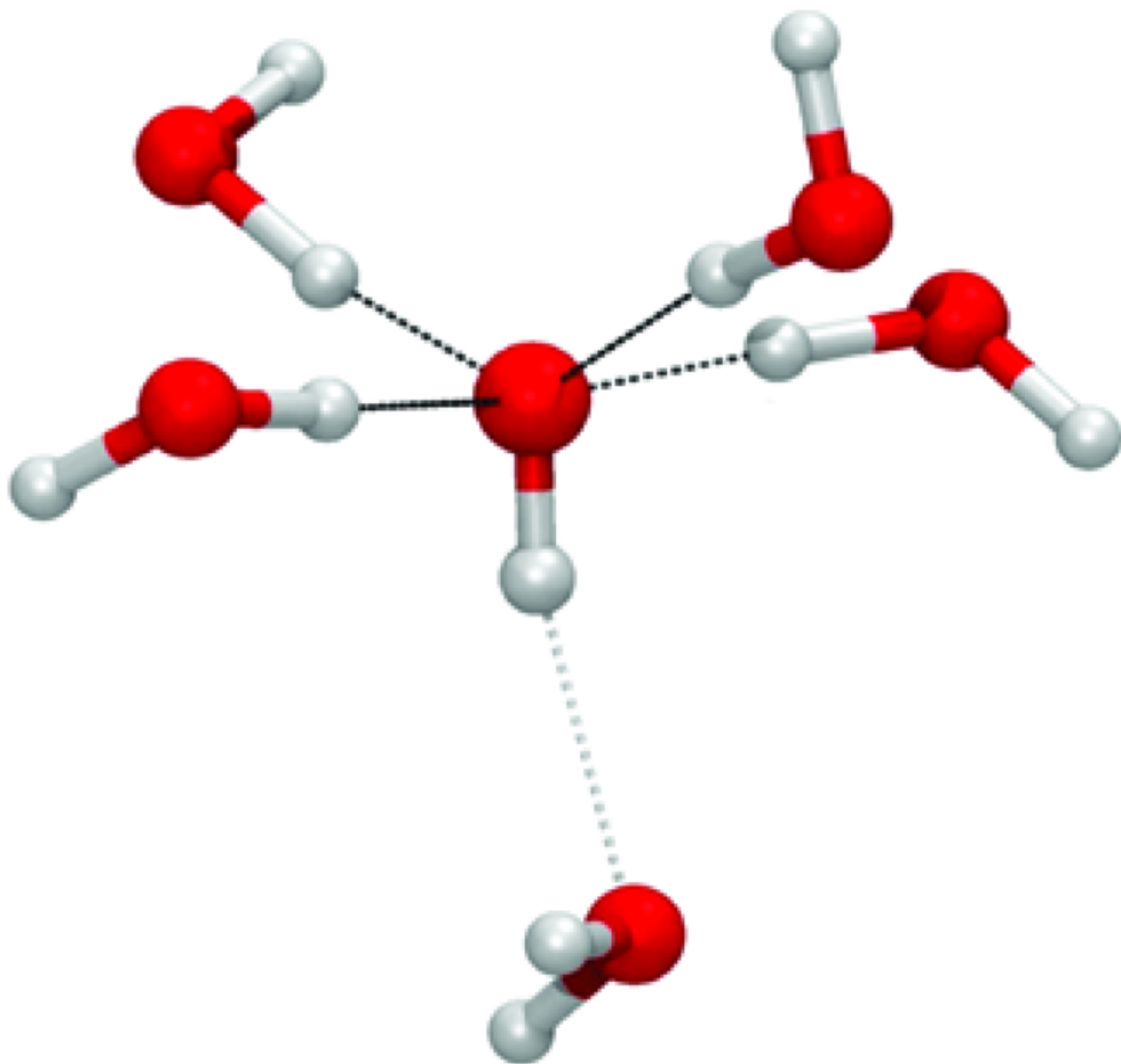
Figure 2: photovoltaic

Figure 3: silica

Figure 4: hydroxide