**Grant Number**: Royal Society International Exchanges Award IES\R3\183166, MIUR-PRIN (Grant No. 2017Z55KCW)

**Sponsor:** Institute of Advanced Studies of the University of Birmingham, Royal Society,MIUR-PRIN

**Project title**: Clear Pathways to Colloidal Diamond

The following files have been archived:

|  |  |
| --- | --- |
| **File name** | **File description** |
| Figure2.zip | Zipped directory containing the data from Monte Carlo simulations of the self-assembly of the one-component and two-component systems of tetrahedral patchy particles with narrow patches. Each of the systems have their own subdirectory, which contains directories housing data from each of the temperatures considered. For each temperature, the initial configurations, input file and final configurations are provided, as well as the energy over the course of the simulation. |
| Figure3.zip | Zipped directory containing the data from Monte Carlo simulations of the self-assembly of the one-component and two-component systems of tetrahedral patchy particles with wide patches. Each of the systems have their own subdirectory, which contains directories housing data from each of the temperatures considered. For each temperature, the initial configurations, input file and final configurations are provided, as well as the energy over the course of the simulation. |
| Figure4.zip | Zipped directory containing the chemical potential calculations for the one-component and two-component systems of tetrahedral patchy particles as a function of patch width. Each of the systems have their own subdirectory, which contains directories housing data for each of the patch angles considered. For each patch angle there are two directories – one for the fluid phase and another for the crystal phase. For each phase data is provided from NPT simulations at P=0.03 for different temperatures and at one of the temperatures data is provided for the calculation of a reference free energy. |
| Figure5.zip | Zipped directory containing the free energy calculations for the cubic and hexagonal polytypes of diamond, as formed by the two-component system of tetrahedral patchy particles at pressures of P=0 and P=0.1, as a function of patch width. At each pressure data from NPT simulations are provided as well as data from Einstein crystal simulations in the NVT ensemble performed at the corresponding equilibrium density. Additionally, data is provided for the self-assembly of the two-component system of N=4000 tetrahedral patchy particles. Data is provided for two densities and for a series of patch widths, where for each patch width 25 independent simulations were performed. |
| SI\_Figure2.zip | Zipped directory containing the data from Monte Carlo simulations of the self-assembly of the one-component system of tetrahedral patchy particles with narrow patches at a density of 0.5. Data from each of the temperatures considered is provided. For each temperature, the initial configurations, input file and final configurations are provided, as well as the energy over the course of the simulation. |
| SI\_Figure3.zip | The energy and bonding probability for the one-component and two-component system of tetrahedral patchy particles with wide patches at a density of 0.5. |
| SI\_Figure4.zip | Zipped directory containing the data from Monte Carlo simulations of the self-assembly of the chromatic two-component system of tetrahedral patchy particles with narrow patches at a density of 0.5. Data from each of the temperatures considered is provided. For each temperature, the initial configurations, input file and final configurations are provided, as well as the energy over the course of the simulation. |
| SI\_Figure5.zip | Data is provided for the self-assembly of the two-component system of N=1000,8000 and 16000 tetrahedral patchy particles with a patch half-angle of 20° at a density of 0.5. For each system size 25 independent simulations were performed. |
| code.zip | Code used to perform the Monte Carlo simulations and generate the data mentioned above. The source directory contains the main simulation code, while the analysis code is used to compute the number of rings, bond-orientational order parameters and fraction of cubic and hexagonal diamond and clathrate in the system. |

**Publications**: (based on this data, if any)