

Three-dimensional microscopic numerical model of an icy mantle of an interstellar dust particle

Development of the three-dimensional microscopic off-lattice Monte Carlo model of an icy mantle of an interstellar dust particle is most challenging theoretical task within this project. The task implies development of a complex numerical code from scratch that must simultaneously include simplified yet realistic description of chemical processes on interstellar grains and be computationally efficient. To the time of preparation of this report, we developed an efficient numerical code that allows simulation of the key chemical process in the interstellar medium – the formation of molecular hydrogen on interstellar grains, under a range of physical conditions.

Realistic structure and shape of dust particles is important for accurate modeling of chemistry on dust particles and structure of icy mantles. It is believed that interplanetary and interstellar dust particles have irregular shape and fractal structure. Off-lattice approach can be applied for an approximate study of the morphology (structure) of the particle and the effects associated with it. Thus, the off-lattice modeling of chemical processes on interstellar grains consists of two major steps. First, the fractal grain core must be generated. Second, simulations of chemistry on the generated core must be carried out. In our model local minima on the surface of the core are found by calculating the interaction potential between atoms. The diffusion paths are not predetermined and can be calculated during operation of the code. The simulation algorithm implemented in the developed numerical code is described below.

1) preliminary step (step ‘0’): Setting the initial conditions – gas and dust temperatures, gas density, abundances of chemical species in gas, radii and masses of specific chemical species; counters for t (time), n (number of throws), f (number of created atoms), d (number of desorbed atoms) and m (number of cases of migration) are initiated as zero; generation of initial core (carbon core is used as ‘first layer’, see pic. 1). Code includes information about all kinds of atoms and molecules and reactions with them. For each type of participating species there is information about their abundances in gas and dust phase, radii and masses, charge, average thermal velocity, their number in the system, number of accreted and desorbed species and their unique index. Moreover, this code keeps information about name and color with which particle will be represented on output file. For all reactions there are indexes of participating elements, probabilities of reactions, energy and reaction rates. Each element is considered as an object with unique index and keeps information about its radius, mass, coordinates, desorption rate, migration rate and binding energy.

2) Step 1: Accretion rates are calculated once for each type of element in the system, because in the model temperature is assumed to be constant over time. Accretion rates calculated as (Tielens, 2005):

$$k_{ac} = n * \sigma * v * S(T, T_d), \quad (1)$$

where n – concentration, σ – cross-section of dust grain, v – thermal velocity of molecule, $S(T, T_d)$ – sticking coefficient for corresponding species

During this step code calculates timelines for accretion and desorption using random number generator (Cuppen & Garrod, 2011),

$$\tau_{ac} = -\frac{\ln(X_1)}{k_{ac}}, \quad (2)$$

$$\tau_{des} = -\frac{\ln(X_2)}{k_{des}}, \quad (3)$$

$$\tau_{hop} = -\frac{\ln(X_3)}{k_{migr}}, \quad (4)$$

where X_1 , X_2 and X_3 – evenly distributed random numbers from 0 to 1; k_{des} and k_{hop} desorption and migration rates correspondingly (calculated at the moment of sticking for each atom) (Tielens, 2005):

$$k_{des} = \nu * \exp\left(-\frac{E_b}{T}\right), \quad (5)$$

$$k_{hop} = \nu * \exp\left(\frac{2a}{h} (2mE_b)^{\frac{1}{2}}\right). \quad (6)$$

In eq. 6 and 7 E_b is measured in Kelvins. At this step τ_{ac} is calculated once for each type of element for the whole system, τ_{des} – for each atom individually (a new random number is generated every time), τ_{hop} – individually for each spot of potentially possible migration of atom. Moreover, before calculation timelines of desorption for each atom there is a check out of the ability to desorb in principle (if atom is covered by another atom or not). In the end of calculation, we sort all events by time, choose the fewest one and the event associated with this least time is performed (in our case – accretion, desorption or migration).

3) Step 2: All calculations at this step depend on the result of the previous one.

a) Case of accretion. Counter of created atoms f and number of throws n increase by 1. Time counter t increases by τ_{ac} . Potential migration points are recalculated for all atoms in a region of radius $2.5 \sigma_{max}$ from the point of sticking. At this distance, the interaction force drops below 10% and doesn't make a significant contribution to the potential value. The formation of bonds with other hydrogen atoms is checked, and if there are any, it is believed that a hydrogen molecule has been formed and the desorption for both atoms is initiated.

b) Case of desorption. Counter of throws n and counter of destructed atoms increase by 1, time counter t increases by τ_{des} from step 1. Potential migration points are recalculated for all atoms in a region of radius $2.5 \sigma_{max}$ from the point of sticking.

c) Case of migration. Counter of throws n and counter of migrations increase by 1, time counter t increases by τ_{des} from step 1. Potential migration points are recalculated for all atoms in a region of radius $2.5 \sigma_{max}$ from start and end points of migration. The formation of bonds with other hydrogen atoms is checked, and if there are any, it is believed that a hydrogen molecule has been formed and the desorption for both atoms is initiated. A more detailed description of the search for migration points is given below.

Steps 1 and 2 are repeated until the selected time limit is reached.

Initial core can be generated both spherical and random shape. In case of approximately spherical initial core carbon atoms are located at the minimum points of the potential at the same distance forming a regular lattice. We use type of regular structure from (Garrod, 2013). The code allows to specify any nonzero core size. Amorphous core is formed by random accretion of carbon atoms to the first initial atom. In this case we use the same mechanisms of accretion and calculation of the location of potential wells as with general accretion during the calculations in the code.

The potential of the surface is calculated as follows. Each atom in the system has its own potential value calculated as Lennard-Jones potential (Lennard-Jones, 1924):

$$U(r) = 4 * \varepsilon * \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right], \quad (7)$$

where U – potential value; r – distance; ε – depth of potential well; σ - the distance where the interaction energy becomes zero.

For two interacting atoms potential is calculated as (Ruthven, 1984):

$$U(r) = 4 * \sqrt{\varepsilon_1 \varepsilon_2} * \left[\left(\frac{(\sigma_1 + \sigma_2)}{2r} \right)^{12} - \left(\frac{(\sigma_1 + \sigma_2)}{2r} \right)^6 \right]. \quad (8)$$

All together atoms form the surface potential of a dust grain. Potential in each point of surface is calculated as superposition of the interaction potentials of atoms in a radius $2.5 \sigma_{max}$. σ_{max} is a maximum possible σ in the system.

The total potential at the point is calculated as

$$U = \sum_{i=0}^n U_i(r_i), \quad (9)$$

where U – potential at one point; U_i – interaction potential between two elements; r_i – distance between interacting elements.

Using the developed code, we explored the efficiency of the formation of molecular hydrogen on amorphous and regular carbonaceous dust grains under the condition typical of early stages of star formation. with the results are presented below in Figure 1.

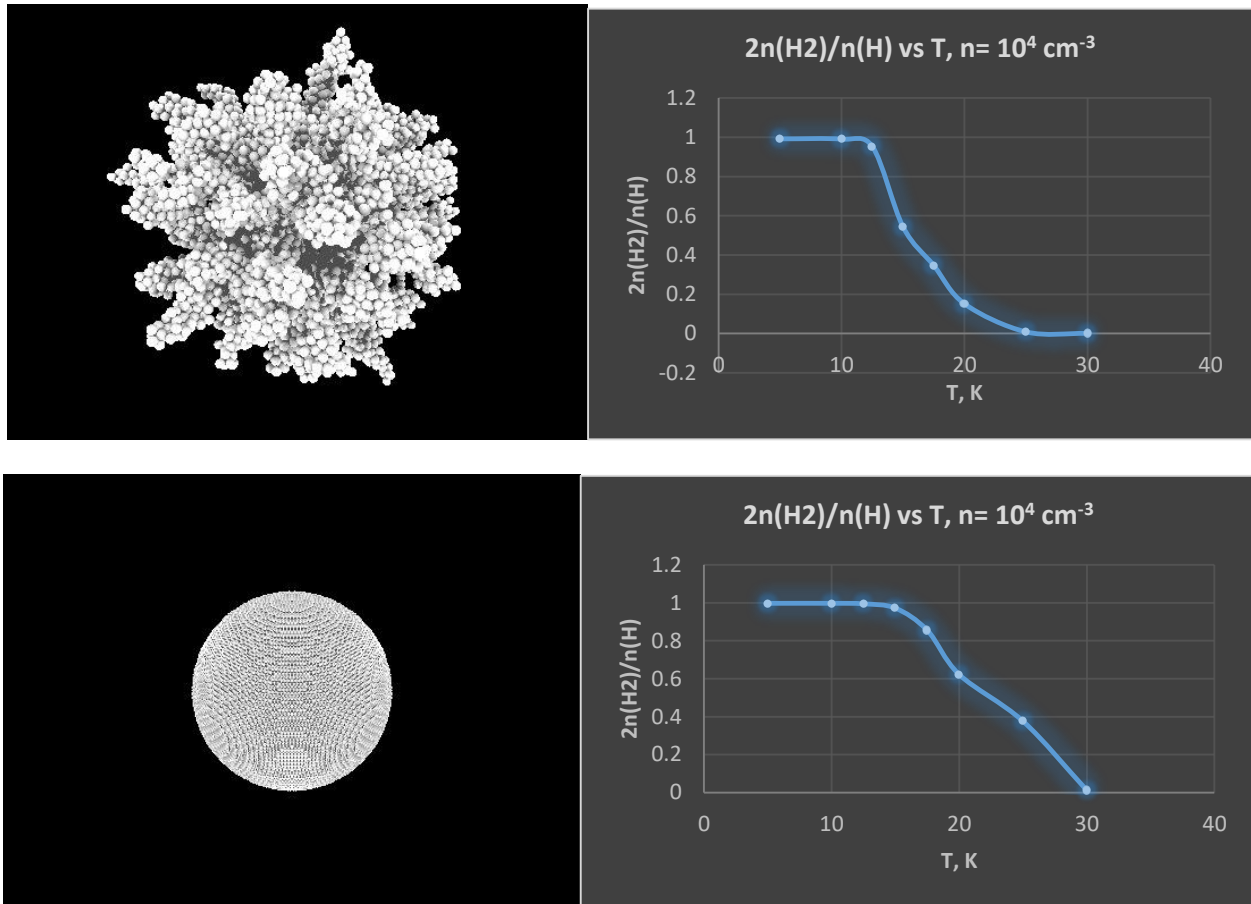


Figure 1. Top left: depiction of a simulated amorphous core of a carbonaceous interstellar dust grain. Top right: the efficiency of atomic hydrogen recombination on the surface of amorphous carbonaceous dust vs. temperature. Bottom left: depiction of a simulated regular spherical carbonaceous interstellar dust grain. Bottom right: the efficiency of atomic hydrogen recombination on the surface of regular spherical; carbonaceous dust vs. temperature

Literature Sources:

1. Tielens A. G. G. M., The physics and chemistry of the interstellar medium. New York: Cambridge University Press – 2005.
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