

COMSOL Multiphysics® Simulation of Chiral Molecule Interaction with Chiral Structures

I. Zabkov¹, V. Klimov², A. Pavlov², D. Guzatov³

¹MIPT, Moscow, Russia

²Lebedev Physical Institute, Moscow, Russia

³Yanka Kupala Grodno State University, Grodno, Belarus

Abstract

Influence of chiral objects on spontaneous emission of atoms and molecules is under attention nowadays. The problem of interaction of chiral molecules with one [1] or two chiral [2] spheres was solved analytically recently by our group. The analytical results however are very difficult and needed to be calculated carefully. We modify the RF Module of COMSOL Multiphysics® in order to simulate numerically interaction of chiral molecules (superposition of electric and magnetic dipoles) with chiral structures. The model was used to confirm results of analytical solution. Moreover for some particular problems calculation with analytical formulas takes more time than numerical simulation with COMSOL Multiphysics®.

Wave equation for chiral media differs slightly from wave equation for usual media. We modified weak form of wave equation together with addition of extra current to satisfy the boundary condition for electric and magnetic fields. From numerical simulation we obtained total, radiative and nonradiative decay rate of chiral molecules in the vicinity of one and two chiral spheres which corresponds to energy irradiated by molecule, outgoing from system molecule + nanoenvironment and absorbed in spheres correspondingly.

Comparison of analytical (solid lines) and numerical results (circles) of chiral molecule situated in the vicinity of one sphere is presented at Figure 1 where dependence of total decay rate versus dimensionless parameter of chirality is shown together with the geometry of the problem. Two molecule orientation as well as two chirality of molecule (left and right) is considered.

Dielectric permittivity of sphere is $\epsilon = 2 + 0.04i$ and magnetic permeability is $\mu = 1$. It can be seen that numerical results are in a good agreement with analytical ones.

As a result, the COMSOL Multiphysics® RF Module was modified in order to work with chiral media. Numerical simulation of interaction of chiral spheres with chiral molecule was obtained and results are in good agreement with analytical ones.

Reference

- [1] Guzatov, D., & Klimov, V. (2012). The influence of chiral spherical particles on the radiation of optically active molecules. *New Journal of Physics*.
- [2] D. Guzatov, V. Klimov, A.A. Pavlov, I. Zabkov, "Radiation of chiral molecule places near dimer of two chiral spheres," (to be published).

Figures used in the abstract

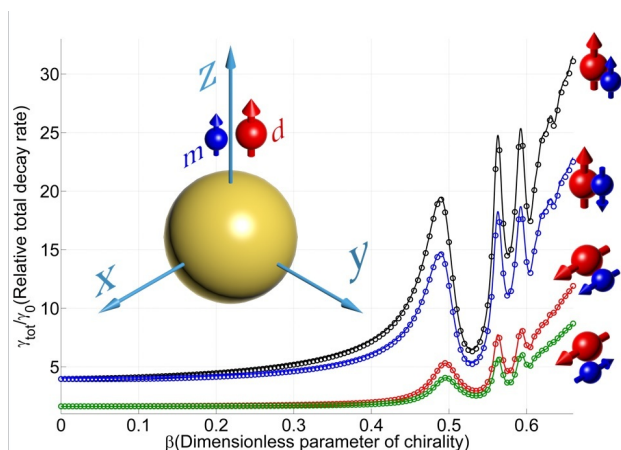


Figure 1: Total decay rate of chiral molecule situated in the vicinity of chiral dielectric sphere versus dimensionless parameter of chirality is shown for 2 orientation of molecule (radial – black and blue lines; tangential – red and green lines) as well as two type of chirality (right – black and red lines; left – blue and green lines). Dielectric permittivity of sphere is $\epsilon=2+0.04i$ and magnetic permeability is $\mu=1$. The geometry of the problem is also shown. Solid line stands for analytical results while circles for results of numerical simulation.