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Computer Modeling of Energy Transfer in Crystal CHRISTOPHER STUETZLE, JOHN COLLINS, MIKE GOUSIE, Wheaton College — The luminescence from impurity ions in ionic crystals is important in terms of its applications to lasers and lamp phosphors, among others. One important process that affects the efficiency of photon emission in these materials is the non-radiative energy transfer among the impurity ions. We have developed a computer program that allows us to investigate the energy transfer process among ions in crystals, and to view the luminescence output from the crystal as a function of time. The user has the ability to model most any crystal structure, and to replace certain ions in the crystal with impurity ions placed either randomly or non-randomly. The probabilities of photon emission and of energy transfer are based on user input. Excitation of the impurities is mimicked by having a portion of the impurity ions "absorb" photons. The program also includes a visualization feature which allows the user to view the periodic nature of the crystal and creates an animation of the energy transfer. We have applied the program to the case of Nd:YAG under several pumping levels, and the results are compared with experimental data.

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