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**Robert D Hill\*** ([rhill19@gmu.edu](mailto:rhill19@gmu.edu)), 13304 Pennypacker Lane, Fairfax, VA 22033. *Modeling complex physical phenomena using energy minimization principle*. Preliminary report.

Modern modeling languages and optimization tools make it possible to analyze complex physical phenomena. The following two examples are driven by the energy minimization principle, and thus can be modeled using optimization: First, we consider a problem of docking a molecular wire to a bacterial photosynthetic reaction center (RC). To assemble efficient photovoltaic devices, it is critically important to explore how to dock highly conducting molecular wires to the RC. Second, we consider the problem of constructing phase diagrams. Phase diagrams illustrate the conditions in which thermodynamically distinct phases (e.g. gas, liquid or solid) can occur in equilibrium for a material or a mixture of materials. We build optimization models for both examples using AMPL and solve them using interior-point method and sequential quadratic optimization technique. (Received September 20, 2010)