THEORETICAL STUDIES OF THE ELECTROSTATIC PROPERTIES OF THE EYE-LENS PROTEIN GAMMA-B CRYSTALLIN. K. Michael Martini, Anthony Harkin, David S. Ross, and George M. Thurston*, Department of Physics and School of Mathematical Sciences, kmm9288@rit.edu, aahsma@rit.edu, dsrsma@rit.edu, georgemthurston@gmail.com.

In previous work we have characterized how interactions between eye lens Gamma-B crystallin proteins change rapidly from attractive to repulsive as protein charge is increased. With the aim of understanding this behavior quantitatively, we are working towards developing electrostatic models of interprotein interactions. We are studying both simplified quantitative models of protein electrostatics, including the Linderstrom-Lang and Tanford-Kirkwood models, as well as detailed partial differential equation models of the electrostatic potential in the vicinity of proteins. These models use the linearized Poisson-Boltzmann equation in regions exterior to the protein. Calculations using the public software Adaptive Poisson Boltzmann Solver (APBS) and the program pdb2pqr at various pH values of Gamma-B crystallin closely matched its measured titration curve. Key issues that need to be addressed for accurately modeling interprotein electrostatic interactions, including charge regulation, will be discussed.