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Non-covalent interactions between ATP and RecA DNA-repairing proteins: DFT and semiempirical calculations[1] JORGE RODRIGUEZ, Department of Physics and Astronomy, Purdue University — The role of Bacterial RecA in the structural maintenance of genomes and the genetic information they carry has been established. In particular, the RecA DNA-repairing protein from *D. Radiodurans*, a radiation-resistant bacteria, is crucial for the repair of double strand breaks (DSBs). We have performed semi-empirical free-energy calculations and QM/MM calculations to study their non-covalent interactions with ATP and ADP. Such studies provide insight into the mechanisms of ATP/ADP $\rightarrow$ RecA energy transfer and, therefore, about specific functional uses of incoming energy for DNA repairing mechanisms. We present a detailed analysis of the non-covalent interactions which minimize the interaction Gibbs free energies leading to the most stable non-covalent binding sites. Van der Waal, hydrogen bonding and electrostatic interactions has been quantified which provides a detailed insight into the mechanisms of ATP-RecA interaction. Further, possible chemical interactions and functional roles of RecA proteins are explored based on the previously mentioned studies. *Acknowledgements*: Funded, in part, by DTRA award 106339 (JHR). Dr. Mark C. Palenik and Mrs. Lora Beard are gratefully acknowledged

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