

NSF EPSCoR

Computational Chemistry
Cluster

Members

- Jerzy Leszczynski (JSU)
- Steven Davis (Ole Miss)
- Ming-Ju Huang (JSU)
- David Magers (MC)
- Ras Pandey (USM)
- Svein Saebo (MSU)
- Gregory Tschumper (Ole Miss)
- John Watts (JSU)

Highlights from Year 2

- 74 publications
- 143 presentations
 - More than 110 by students
 - Almost 50 by undergraduates
- 18 invited lectures
- 21 grants submitted – 11 already funded

Students

- 20 graduate students
- 28 undergraduate students
- 3 post docs

Jerzy Leszczynski's Group Graduate Students



Reeshemah Allen Tomekia Simeon Teri Robinson

Julia Saloni Jaroslaw Szymczak



Olexandr Isayev Gareth Forde Glake Hill



Post-Doc.
Dr. Yevgeniy Podolyan

Undergraduate Students



1. Angela Fortner 2. Chi-Cobi Speaks 3. Tiffarah Cline 4. Demarcio Reed

5. Stephanie Daniels
6. Andrea Sterling
6. Cynthia Jeffries



Tschumper Research Group, Summer 2003

Julie Anderson, **Kelly Crager**, Jennifer Chapman ,
Abby Jones, **Lisa Fedoroff**, Aimee Zaiontz

Brian Hopkins, Greg Tschumper, Anne Paige Tschumper, Sam Tyagi, Adel Elsohly



Tschumper Research Group Spring 2004

Front Row:

Abby Jones and
Julie Anderson

Back Row:

Adel Elsohly,
Brian Hopkins, and
Greg Tschumper

MC Computational Chemistry Group SERMACS 2003 in Atlanta



Jeanann Lovell, Shelley Huskey, Patricia Honea, David Magers, Jami Lewis, Ashley Ringer, and Crystal Coghlan

MC Computational Chemistry Group MAS 2004 in Biloxi

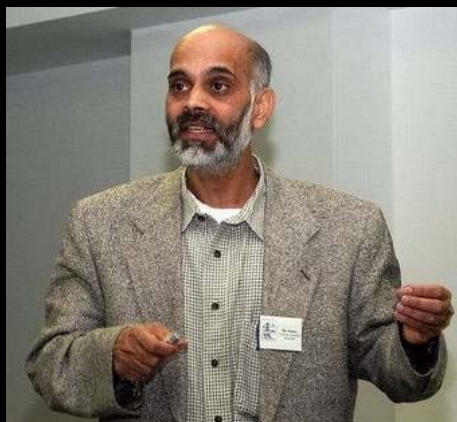


Jeanann Lovell, Patricia Honea, Shelley Huskey, David Magers, Ashley Ringer, Crystal Coghlan, and Jami Lewis

Big Events of the Past Year

- 12th Conference on Current Trends in Computational Chemistry in Jackson, October 31- November 1, 2003
- 4th Southern School on Computational Chemistry in Orange Beach, AL, March 26-27, 2004
 - Serves as the location of our annual review by Advisory Panel
- Summer Institute at JSU (June – July, 2003)

Some Scenes from the 4th SSCC



Some of Our Research Progress

- Developed algorithms based in graph theory to predict products in chemical reactions.
- Implemented parallel code for MP2 analytic gradients
- Developed QM/MM methods to characterize weak interactions in large systems.
- Modeled thin film growth by computer simulation by considering a mixture of hydrophobic, polar, and aqueous components in an effective solvent medium with appropriate interactions and molecular weights.
- Presented evidence that the CCSD(T) method is not sufficient to determine pi-pi stacking energies to sub-chemical accuracy.

Some of Our Research Progress (cont.)

- For the first time, the physical nature of intermolecular interactions between 10 DNA stacked bases was examined by an interaction energy decomposition method based on the variation–perturbation theory. The electrostatic multipole component closely showed the trend of total interaction energy in all considered systems.
- The deamination of cytidine performed by cytidine deaminase was modeled using DFT methods. This study allowed for the first time to close the complete reaction cycle for the investigated process.
- Ground and excited state properties of hypoxanthine were studied using the single and multi-reference methods. The geometry of the molecule was found to be highly nonplanar in the lowest singlet $\pi\pi^*$ excited state and approximately planar in the lowest singlet $n\pi^*$ state, except for the CO group which was displaced appreciably out-of-plane from the ring plane.

Some of Our Research Progress (cont.)

- The *gem*-dimethyl effect was characterized to be at least somewhat a thermodynamic effect by computing conventional strain energies of cyclobutane, methylcyclobutane, and 1,1-dimethylcyclobutane.
- The selectivity of binding to triplex DNA by several naphthylquinoline derivatives was shown to depend on the flexibility of the side chain.
- Certain intermediates in the base hydrolysis of TNT were characterized by computation of UV-Vis spectra.
- The stabilizing effect of σ -delocalization in cyclopropane was demonstrated by conventional strain energy calculations of silacyclopropane and silacyclobutane.

Some of Our Research Progress (cont.)

- Calculated the strain energies of cycloalkapolyenes with *trans* double bonds.
- Contrary to previous semi-empirical studies, *ab initio* and DFT studies have shown that 9 β -fluoroprednisolone is more stable than 6 β -fluoroprednisolone.
- Interpreted the UV spectrum of methylhydroperoxide and its photodissociation by CCSD(T) calculations.
- CCSD(T) calculations with extended atomic natural orbital basis sets with both UHF and ROHF reference functions have yielded results for iron(II) trichloride anion that are consistent with experimental data.

Planned Events for the Coming Year

- 13th Conference on Current Trends in Computational Chemistry in Jackson, November 12-13, 2004
- 5th Southern School on Computational Chemistry in Orange Beach, AL, March, 2005
- Summer Institute at JSU (June – July, 2004)
 - Broader involvement by cluster members planned
- Start developing a web site with computational chemistry tutorials
- Submit a collaborative equipment grant to NSF