

Computational Chemistry Symposium in Honor of John Pople

Room: FH-133

Monday 8:30AM - 4:55PM

Larry Curtiss, Organizer, Presiding (morning)

- 8:30 Opening Remarks
- 236.** 8:35 QUANTUM CHEMICAL MODELS. **John A. Pople**¹; ¹Weinberg College of Arts and Sciences, Northwestern University, 2145 Sheridan Road, Evanston Campus 3113, Evanston, Illinois
- 237.** 9:10 QUANTUM CHEMICAL MODELS FOR ACCURATE THERMOCHEMISTRY: RECENT ADVANCES. **Krishnan Raghavachari**¹; ¹Indiana University Bloomington, Professor, Department of Chemistry, Indiana University, Bloomington, IN
- 238.** 9:45 IMPROVED BASIS SETS FOR CBS EXTRAPOLATIONS. **George A. Petersson**¹; ¹Wesleyan University, Chem Dept, Middletown, Connecticut, US
- 10:20 Break
- 239.** 10:45 COMPUTATIONAL THERMOCHEMISTRY - FROM THE GAS PHASE TO SOLUTION. **David Adams Dixon**¹; ¹Pacific Northwest National Laboratory, Pacific Northwest National Laboratory, Fundamental Science Division MS K9-90, Richland, WA
- 240.** 11:20 A GEMINAL MODEL CHEMISTRY. **Vitaly Rassolov**¹; ¹Science and Mathematics, University of South Carolina, 631 Sumter St, Columbia, SC
- 11:55 Lunch
- George Schatz, Presiding (afternoon)
- 241.** 1:30 AB INITIO VS. SEMIEMPIRICAL MOLECULAR ORBITAL THEORIES. **Karl F. Freed**¹; ¹University of Chicago, 5801 South Ellis Avenue, University of Chicago, Chicago, IL
- 242.** 2:05 WHAT DETERMINES THE SIGN OF THE FERMI-CONTACT CONTRIBUTION TO THE TOTAL NMR SPIN-SPIN COUPLING CONSTANT. **Janet E. Del Bene**¹; ¹Youngstown State University, Department of Chemistry, Youngstown, OH
- 243.** 2:40 ENDOHEDRAL MOTIONS OF METAL CATIONS INSIDE SINGLE-WALLED CARBON NANOTUBES. **Jerzy Cioslowski**¹; ¹Florida State University, Chemistry building, Tallahassee, FL, US
- 3:15 Break
- 244.** 3:45 THEORETICAL STUDIES OF THE ADDITION OF H ATOM TO ETHYLENE AND ACETYLENE. **Lawrence Harding**¹, **Albert Wagner**¹; ¹Argonne National Laboratory, Chemistry Division, Argonne National Laboratory, Argonne, IL
- 245.** 4:20 INTERFACE BETWEEN MOLECULES AND METALS: SOME NOTIONS. **Mark A. Ratner**¹, **Harold Basch**¹; ¹Weinberg College of Arts and Sciences, Northwestern University, 2145 Sheridan Road, Northwestern University, Evanston, Illinois