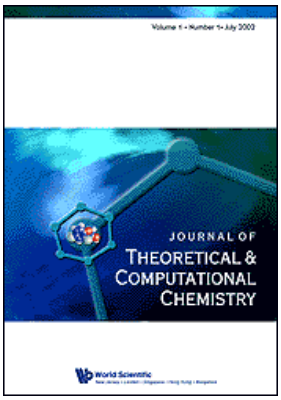
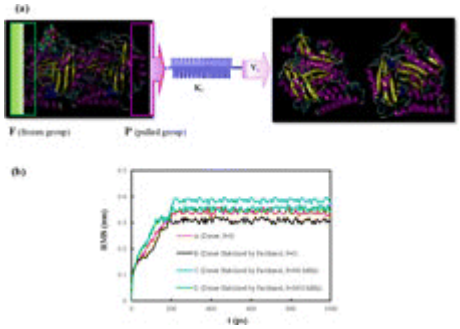
Journal of Theoretical and Computational Chemistry

Volume: 15, Number: 02 (March 2016)

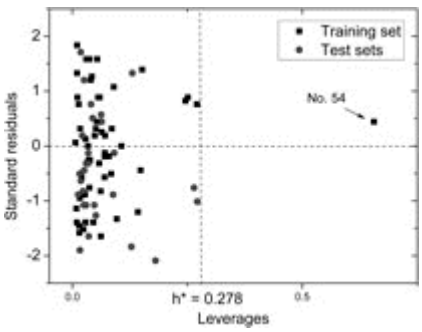


RESEARCH PAPERS

• Effects of external electric fields of 900 MHz and 2450 frequencies on *αβ*-tubulin dimer stabilized by paclitaxel, have been simulated vai the molecular dynamics method.
• Stabilizing dimer by paclitaxel leads to more structural rigidity.
• Application of electric field of 2450MHz does not decrease the rigidity of the systems as much as application of electric field of 900MHz frequency.



• An accurate QSPR for Tgs of 82 polyacrylates was developed.
• Molecular descriptors were calculated from the motion units.
• Calculating molecular descriptors from the motion units is feasible.

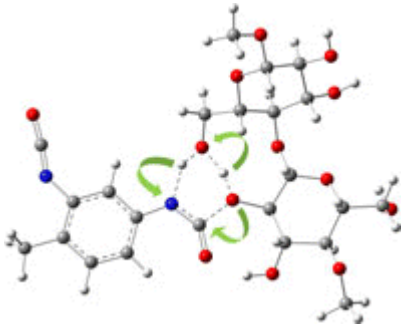


3. **A DFT study on the mechanism of reaction between 2, 4-diisocyanatotolune and cellulose**

Jiping Cao, Yali Liu, Aijuan Shi, Yuan Yuan, Mingliang Wang

1650012

The reaction mechanisms between 2, 4-Diisocyanatotolune and cellulose have been investigated using the density functional theory at the B3LYP/6-31+G(d, p). The calculations show that the direct addition of 2, 4-TDI and cellulose possesses an unrealistically high barrier of 32~34 kcal · mol^{-1}. With a neighboring *β*-D-glucose unit serving as hydrogen transporter, the reaction energy barrier is significantly reduced to 16~18 kcal · mol^{-1}, which is in a good accordance with the experimental activation energy of 13.9~16.7 kcal · mol^{-1}.

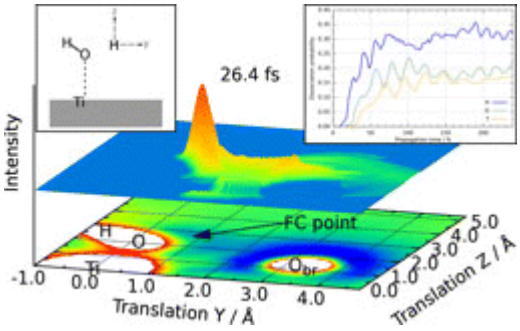


4. **Photodissociation of water on rutile (110): A wave packet approach based on first principles**

Jan Mitschker, Thorsten Klüner

1650013

The photodissociation of water on a rutile (110) surface has been studied with ab initio methods in combination with numerical wave packet propagation. Ground and an electronically excited state were calculated on a CASSCF level of theory. Quantum dynamical simulations reveal a significant isotope effect caused by the topology of the PES near the Franck–Condon point.

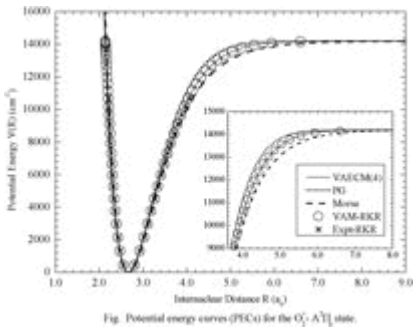


5. **High-lying vibrational energies and analytical potential energy functions for some electronic states of diatomic ions**

Chun Guo Zhang, Qun Chao Fan, Zhi Xiang Fan, Hui Dong Li, Jia Fu

1650014

• We find the analytical potentials of other methods may show the unphysical tiny barriers in the asymptotic and dissociation region.
• We modify our variational algebraic energy consistent method (VAECM) to adapt to different diatomic ions.
• Modified VAECM(4) can obtain the full vibrational spectra and give accurate analytical potential energy functions for diatomic ions.

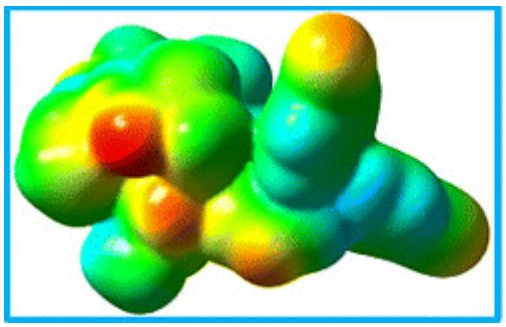


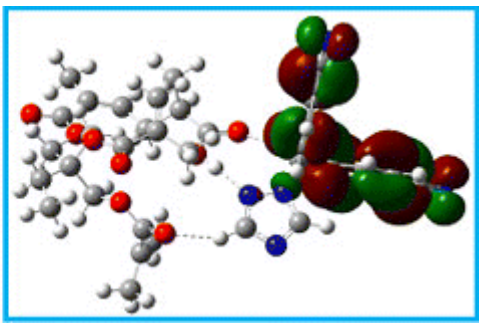
6. **DFT computations on the hydrogen bonding interactions between methacrylic acid-trimethylolpropane trimethacrylate copolymers and letrozole as drug delivery systems**

Saeedeh Kazemi, Aliasghar Sarabi Daryani, Majid Abdouss, Zahra Shariatinia

1650015

DFT computations were performed on the interactions of letrozole drug with three copolymers. It was found that all of the copolymer-drug interactions were exergonic and exothermic. According to the most negative values of $\Delta E_{binding}$, $\Delta G_{interaction}$ and $\Delta H_{interaction}$, complexes **7** and **8** (among two particles systems) as well as complex **13** (among three particles systems) were suggested as the most promising drug delivery systems.



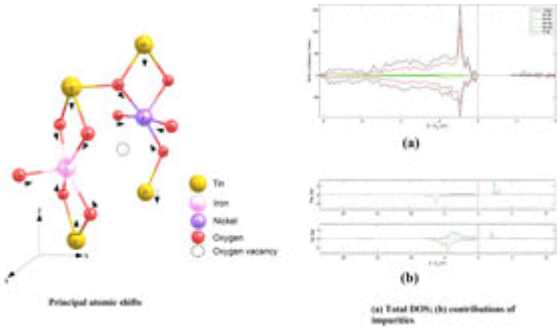


7. **A quantum-chemical approach to Ni and Fe codoping in SnO_2**

Arvids Stashans, Alexander Chamba

1650016

Density functional theory study of oxygen vacancy and two transition metal impurities, Fe and Ni, in SnO_2 material has been conducted. The lowest energy configuration is found when the Ni impurity finds itself at the closest position, 2.18 Å, with respect to the oxygen vacancy and the Fe-Ni interatomic distance is about 4.04 Å. Local magnetic moment occurring for this configuration is due to the contributions of Ni 3*d*, Fe 3*d* and impurity-closest O 2*p* states.

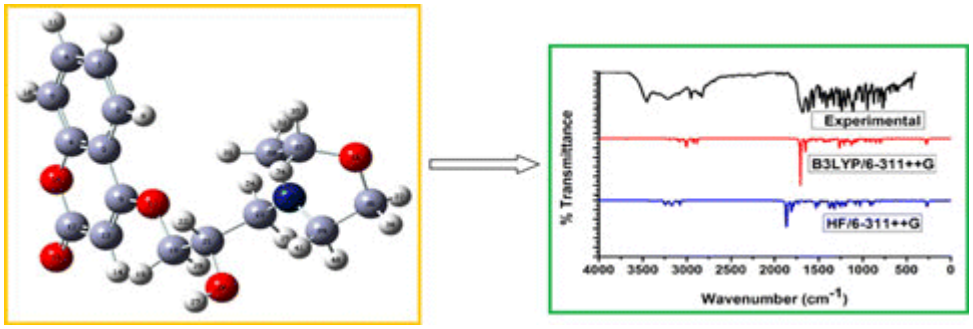


8. **Combined experimental and theoretical studies on 4-(2-hydroxy-3-morpholin-4-yl-propoxy)-chromen-2-one**

Priyanka, Sanjay Kumar Srivastava, Diksha Katiyar

1650017

Complete assignments of vibrational modes have been made using HF and DFT/B3LYP methods with 6-311++G basis set. The ^{1}H and ^{13}C NMR chemical shifts were calculated by GIAO method at B3LYP/6-311++G and B3LYP/6-311++G(2df,2pd) levels of theory and compared with experimental ones. The UV-vis spectra were examined in ethanol and water solutions and calculated using TD-DFT approach.



9. Microsolvation of CH^+ in helium: An *ab initio* study

Mohammad Solimannejad, Behnia Sadat Mirhoseini, Mehdi D. Esrafili

1650018

Microsolvation and interaction of the CH^+ cation with $He_{n=1-11}$ clusters are reported at MP2/aug-cc-pVTZ and QCISD/aug-cc-pVTZ levels. The results of this study have determined the existence of eleven distinct ligand which leads to the formation of three shells. The attractive polarization and dispersion components make the major contribution to the stability of studied complexes.