

List of Publications

Related to thesis

- [1] **Bhattacharjee, D.**, Mishra, B. K. and Deka, R. C. Effect of double aluminium doping on the structure, stability and electronic properties of small gold clusters. *Journal of Materials Science*, 50:4586-4599, 2015.
- [2] **Bhattacharjee, D.**, Mishra, B. K. and Deka, R. C. Theoretical insight on atmospheric chemistry of HFE-365mcf3: reactions with OH radicals, atmospheric lifetime, and fate of alkoxy radicals ($\text{CF}_3\text{CF}_2\text{CH}(\text{O}^\bullet)\text{OCH}_3/\text{CF}_3\text{CF}_2\text{CH}_2\text{OCH}_2\text{O}^\bullet$). *Journal of Molecular Modeling*, 21:69, 2015.
- [3] **Bhattacharjee, D.**, Mishra, B. K., Chakrabartty, A. K. and Deka, R. C. Catalytic activity of anionic Au–Ag dimer for nitric oxide oxidation: a DFT study. *New Journal of Chemistry*, 39:2209-2216, 2015.
- [4] **Bhattacharjee, D.**, Mishra, B. K. and Deka, R. C. A DFT study on structure, stabilities and electronic properties of double magnesium doped gold clusters. *RSC Advances*, 4:56571-56581, 2014.
- [5] Deka, R. C., **Bhattacharjee, D.**, Chakrabartty, A. K. and Mishra, B. K. Catalytic oxidation of NO by Au_2^- dimers: a DFT study. *RSC Advances*, 4:5399-5404, 2014.
- [6] **Bhattacharjee, D.**, Mishra, B. K., Chakrabartty, A. K. and Deka, R. C. DFT and QTAIM studies on structure and stability of beryllium doped gold clusters. *Computational and Theoretical Chemistry*, 1034:61-72, 2014.
- [7] Mishra, B. K., Gour, N. K., **Bhattacharjee, D.** and Deka, R. C. Atmospheric chemistry of HFE-7000 ($i\text{-C}_3\text{F}_7\text{OCH}_3$) and isofluoro-propyl formate ($i\text{-C}_3\text{F}_7\text{OC}(\text{O})\text{H}$): reactions with OH radicals, atmospheric lifetime and fate of alkoxy radical ($i\text{-C}_3\text{F}_7\text{OCH}_2\text{O}^\bullet$)—a DFT study. *Molecular Physics*, 114:618-626, 2016.

Other related publications

- [8] Mohan, S. C., **Bhattacharjee, D.**, Deka, R. C. and Jothivenkatachalam, K. Combined experimental and theoretical investigations on the encapsulation of nickel (II) tet-a complex in zeolite Y and its photocatalytic activity. *RSC Advances*, 6:71214-71222, 2016.
- [9] **Bhattacharjee, D.**, Tiwari, L., Singh, H. J., Mishra, B. K. and Deka, R. C. Theoretical investigation on mechanism, kinetics and thermochemistry of gas-phase reactions of ethyl trifluoroacetate with OH radicals. *Journal of Fluorine Chemistry*, 178:79-85, 2015.
- [10] Deka, P., **Bhattacharjee, D.**, Sarmah, P., and Deka, R. C., and Bharali, P. Catalytic reduction of water-contaminant '4-nitrophenol' over manganese oxide supported Ni nanoparticles. In Kurisu, F., Ramanathan, A., Kazmi, A. A., and Kumar, M., editors, *Trends in Environmental Science and Technology*, pages 35-48. Capital Publishers, New Delhi and co-published by Springer International Publishing, Cham, Switzerland, 2017.
- [11] Begum, P., **Bhattacharjee, D.**, Mishra, B. K. and Deka, R. C. Density functional study on structures, stabilities, and electronic properties of size-selected Pd_nSi^q ($n= 1-7$ and $q= 0,+ 1,- 1$) clusters. *Theoretical Chemistry Accounts*, 133:1418, 2014.
- [12] Mishra, B. K., Chakrabartty, A. K., **Bhattacharjee, D.** and Deka, R. C. Theoretical investigation on unimolecular decomposition of malonic acid: a potential sink for ketene. *RSC Advances*, 4:38034-38039, 2015.
- [13] Sar, D., Bag, R., **Bhattacharjee, D.**, Deka, R. C. and Punniyamurthy, T. Iron (III)-Mediated Radical Nitration of Bisarylsulfonyl Hydrazones: Synthesis of Bisarylnitromethyl Sulfones. *The Journal of Organic Chemistry*, 80:6776-6783, 2015.
- [14] Mishra, B. K., Chakrabartty, A. K., **Bhattacharjee, D.** and Deka, R. C. Theoretical study on the kinetics and branching ratios of the gas phase reactions

- of 1, 1-Dichlorodimethylether (DCDME) with Cl atom. *Structural Chemistry*, 24:1621-1626, 2015.
- [15] Mishra, B. K., Lily, M., Chakrabartty, A. K., **Bhattacharjee, D.**, Deka, R. C., and Chandra, A. K. Theoretical investigation of atmospheric chemistry of volatile anaesthetic sevoflurane: reactions with the OH radicals and atmospheric fate of the alkoxy radical $(CF_3)_2CHOCHFO$: thermal decomposition vs. oxidation. *New Journal of Chemistry*, 38:2813-2822, 2014.
- [16] Chakrabartty, A. K., Mishra, B. K., **Bhattacharjee, D.** and Deka, R. C. Mechanistic and kinetics study of the gas phase reactions of methyltrifluoroacetate with OH radical and Cl atom. *Molecular Physics*, 111:860-867, 2013.
- [17] Chakrabartty, A. K., Mishra, B. K., **Bhattacharjee, D.** and Deka, R. C. Theoretical study on the kinetics and branching ratios of the gas phase reactions of 4, 4, 4-trifluorobutanal (TFB) with OH radical in the temperature range of 250–400K and atmospheric pressure. *Journal of Fluorine Chemistry*, 154:60-66, 2013.