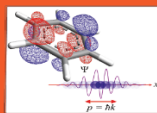


Abstract

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Bangladesh Association for Computational and Materials Science



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Metal-organic frameworks, (MOFs) for water sorption for cycling heat transformation processes

Abstract

Water-stable MOFs with suitable water uptake capacity are gaining attention for reversible cycling water sorption in order to achieve low temperature heat transformation applications in adsorption heat pumps (AHPs), following our first report [1]. AHPs may be alternatives or supplements to conventional compression systems operating with high input of electricity. By using low grade heat as the driving energy, AHPs can significantly help to minimize electricity consumption. AHPs are based on the evaporation and consecutive adsorption of coolant liquids, preferably water (Figure 1a). The process is driven and controlled by the microporosity and hydrophilicity. Yet, the specific temperature boundaries for evaporation, desorption, heat rejection temperature from the adsorbent and the condenser for a desired cycling water sorption application necessitate the tailoring of the adsorbent in terms of hydrophilicity/hydrophobicity for optimized working conditions, which we have addressed here with a mixed-linker concept of MOF-160/CAU-10-H (Figure 1b) [2]. Further, for applications of MOFs one of the biggest current issues is to find effective methods to shape these microcrystalline, powdery materials into manageable forms such as monoliths, pellets or surface coatings with sufficient mechanical and chemical stability, maximal bulk density etc. under preservation of the crucial MOF porosity properties. We have approached this task successfully with MOF@polymer in different binder composites under retention of MOF porosity and hydrophilicity (Figure 1c,d) [3].

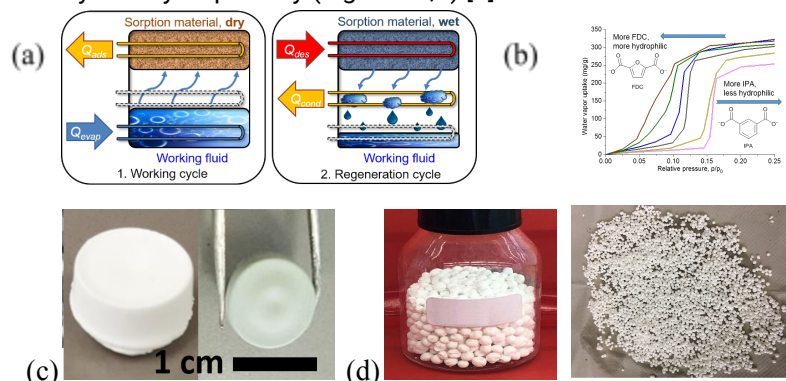


Figure 1. (a) Schematic illustration of the principle of adsorption heat pumps with the useful/needed enthalpies. (b) Hydrophilicity tuning through the transition of a mixed-linker Al-based MOF from MIL-160 to CAU-10-H. (c) Shaping of MOFs with polymers into mechanically stable monoliths and (d) shaping of MOFs into robust 1-2 mm diameter grains under retention of MOF porosity.

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Efficiently Tailoring Polyethylenes using Late Transition Metal Precatalysts

Abstract

It has been argued about what is the sustainable polymer. Polyolefin, indeed, answered by professional scientists. Beyond traditional polyolefin materials based on titanium,¹ chromium² and vanadium catalysts³, scientists have considered of microstructures of polymeric materials developed by late transition metal complexes precatalysts initiated by Brookhart^{4,5a} and Gibson^{5b} with extensive works.⁶ The unique properties and microstructures could be described as either highly linear polyethylenes using iron (and cobalt) precatalysts^{7,8} or highly branched polyethylenes using nickel.^{8,9} In our pursuing novel models of the precatalysts, it is necessary for us to make elegant organic strategies of ligand frameworks,¹⁰ through developing new ruthenium catalyst. Interestingly the catalyst could perform multi-purposes to facilitate the formation of such *N*-heteroatom-containing cyclic compounds as well as the transformation of biomass into fine chemicals.¹¹ In general, we are working on developing novel catalytic systems for fundamental research as well as industrial application.

Acknowledgements: The work supported by the National Nature Science Foundation of China (No. 21871275 and 51861145303) and the Innovated Cultivation Project of ICCAS (CXPY-19).

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Development of novel antibiotics that dysregulate the ClpP protease

Abstract

Evolving antimicrobial resistance has motivated the search for novel targets and alternative therapies. Caseinolytic protease (ClpP) has emerged as an enticing new target since its function is conserved and essential for bacterial fitness, and because its inhibition or dysregulation leads to bacterial cell death. ClpP protease function controls global protein homeostasis and is, therefore, crucial for the maintenance of the bacterial proteome during growth and infection. Previously, acyldepsipeptides (ADEPs) were discovered to dysregulate ClpP, leading to bactericidal activity against both actively growing and dormant Gram-positive pathogens. Unfortunately, these compounds had very low efficacy against Gram-negative bacteria. Hence, we sought to develop non-ADEP ClpP-targeting compounds with activity against Gram-negative species and called these activators of self-compartamentalizing proteases (ACPs). These ACPs bind and dysregulate ClpP in a manner similar to ADEPs, effectively digesting bacteria from the inside out. We performed further ACP derivatization and testing to improve the efficacy and breadth of coverage of selected ACPs against Gram-negative bacteria. We observed that a diverse collection of *Neisseria meningitidis* and *Neisseria gonorrhoeae* clinical isolates were exquisitely sensitive to these ACP analogs. Furthermore, based on ACP-ClpP cocrystal structure solved here, we demonstrate that ACPs could be designed to be species specific. This validates the feasibility of drug-based targeting of ClpP in Gram-negative bacteria.



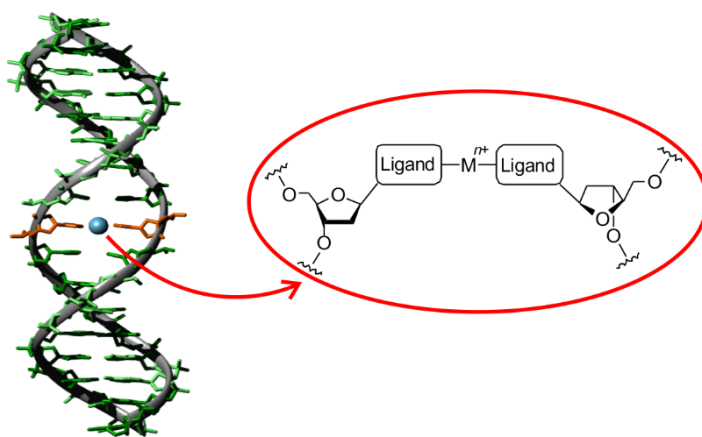
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DNA with Metal-Mediated Base Pairs

Abstract

Due to their predictable self-assembly and their ease of modification, nucleic acids represent an important building block in nanotechnology.^[1] As a result of their polyanionic nature, they always occur in combination with metal ions. A site-specific functionalization of nucleic acids with (transition) metal ions by using ligand-based nucleosides enables the formation of artificial nucleic acids with metal-based functionality and thereby extends their applicability significantly. The resulting metal-mediated base pairs (see figure) are at the focus of our research in this field of bioinspired supramolecular coordination chemistry.^[2] This lecture will summarize our efforts in the previous decade to establish metal-mediated base pairs and to understand better the principles of their formation, starting with the imidazole–Ag(I)–imidazole pair,^[3] but also encompassing dinuclear metal-mediated base pairs^[4] and the light-triggered formation of metal-mediated base pairs.^[5]



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Intermediate band solar cells based on highly-mismatched ZnTeO alloy semiconductors

Abstract

Highly mismatched alloys are a class of materials whose fundamental properties are dramatically modified through the substitution of a relatively small fraction of host atoms with an element of very much different electronegativity. In ZnTe, the incorporation of a small amount of isoelectronic O leads to the formation of a narrow, O-derived intermediate band (IB, E_i) located well below the conduction band (CB, E_c) edge of the ZnTe through an anticrossing interaction between localized states of O and the CB of the ZnTe matrix. Therefore, ZnTe_{1-x}O_x (ZnTeO) alloy is one of the potential candidates for an absorber material in a bulk intermediate band solar cell (IBSC). Here, we review our recent progress on the development of ZnTeO based IBSCs using n-ZnS window layer and Cl-doped ZnTeO. With n-ZnS window having a smaller conduction band offset with ZnTe, the open circuit voltage of ZnTeO IBSC was improved. Cl-doping was performed to introduce electrons into the IB of ZnTeO that is required to be half-filled with electrons for the efficient operation of an IBSC. Low temperature photoluminescence spectra indicated that the doped Cl atoms act as donors in ZnTeO. The improved photocurrent induced by two-step photon absorption was demonstrated in the IBSC using Cl-doped ZnTeO. These results clearly indicate that the Cl-doping into ZnTeO and the use of n-ZnS window are effective to improve the properties of ZnTeO-based IBSC.



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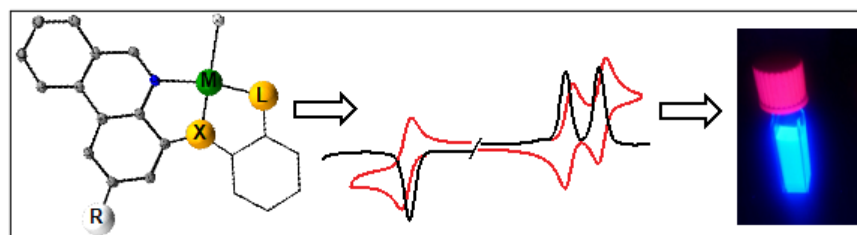
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Benzannulated Aromatic N-Heterocycles and their Coordination Complexes

Abstract

Pyridines appear prominently in a number of well-known "non-innocent" ligand systems, participating both 'directly' and 'indirectly' in the redox and chemical reactivity of metal complexes. 'Benzannulation' can be used to extend the conjugated system of pyridine to quinoline (2,3-benzopyridine) to acridine (2,3-benzoquinoline), stabilizing the lowest unoccupied molecular orbital (LUMO) of the molecule while raising the energy of the highest occupied molecular orbital (HOMO). In the context of coordination complexes, this should introduce more energetically accessible, vacant orbitals and stronger metal-ligand bonding, and therefore can enable more facile chemical and redox non-innocence. To test this hypothesis, we developed synthetic routes to *phenanthridine* derivatives amenable for inclusion in multidentate ligands. Phenanthridine (3,4-benzoquinoline) is an asymmetric isomer of acridine (2,3-benzoquinoline) with an electronically accessible extended π -system and a chemically accessible, imine-like C=N double bond. These features have led to its application as the core of fluorescent DNA intercalators (ethidium bromide), in advanced chemotherapeutics ('phenanthriplatin'), and as a biomimetic hydride-shuttling co-catalyst in hydrogenation reactions. In this presentation, the impact of the *site* of π -extension on the materials properties^[1] and chemical reactivity^[4] of benzannulated N-heterocycles and their coordination complexes will be discussed.



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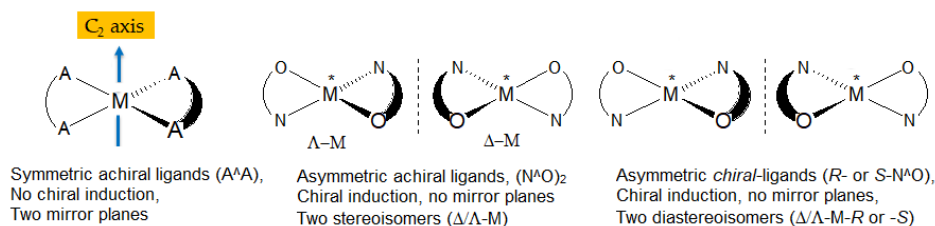
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Diastereoselection and Δ/Λ -chirality induction-at-metal in non-planar four coordinated metal-*chiral* Schiff base complexes: A quantum chemical approach

Abstract

Transition metal complexes with asymmetric ligands ($N^{\wedge}O$) exhibit Δ/Λ -chirality induction at-metal in four-coordinated non-planar complexes with C_2 -symmetry and provide two stereoisomers with opposite configuration at-metal (e.g., Δ -M and Λ -M), while no isomer for symmetric ligands ($A^{\wedge}A$). Uses of asymmetric *chiral*-ligands (R - or S - $N^{\wedge}O$) provide two diastereomers Δ -M(R - $N^{\wedge}O$) and Λ -M(R - $N^{\wedge}O$) (or Λ -M(S - $N^{\wedge}O$) and Δ -M(S - $N^{\wedge}O$)) with one being thermodynamically preferred (Scheme 1).¹⁻¹⁰ X-ray structural analyses, the most reliable and quantitative tools to assign the absolute configuration of the metal centre, suggest only the formation of a single diastereomer Λ -M(R -N,O) or Δ -M(S -N,O) (or *vice versa*) in the enantiopure crystals of pseudotetrahedral $[M(R$ or S -N,O)₂].¹⁻¹⁰ Measurement of only one single crystal structure (reported as the only diastereomer found at solid-state), does not exclude the existence of other diastereomer (may be minor or major) in bulk crystal sample. Due to various *inter*- and/or *intra*-molecular contacts and/or lattice forces, the solid-state preferred structures might not necessarily correspond to thermodynamically stable diastereomer formed in solution or gas phase. ¹H NMR spectra in solution can show up separate/or single peaks for Λ - and/or Δ -diastereomers (if any) and hence, provide both qualitative and quantitative information, showing a dynamic equilibrium between the two diastereomers ($\Lambda \rightleftharpoons \Delta$) as a function of temperature- and/or time.¹⁻¹⁰ Electronic spectra (UV-Vis/ECD) in solution were successfully used to assign electronic/*chiroptical* properties, and to envisage qualitative description of Λ - vs. Δ -form. In fact, combined studies of experimental and calculated ECD spectra by DFT/TDDFT suggest diastereomeric excess of Λ -M- R or Δ -M- S (or *vice versa*) in solution, parallel to a single diastereomer at solid-state or relatively more stable calculated gas phase diastereomer.^{7-10,12-15}



(Scheme 1)

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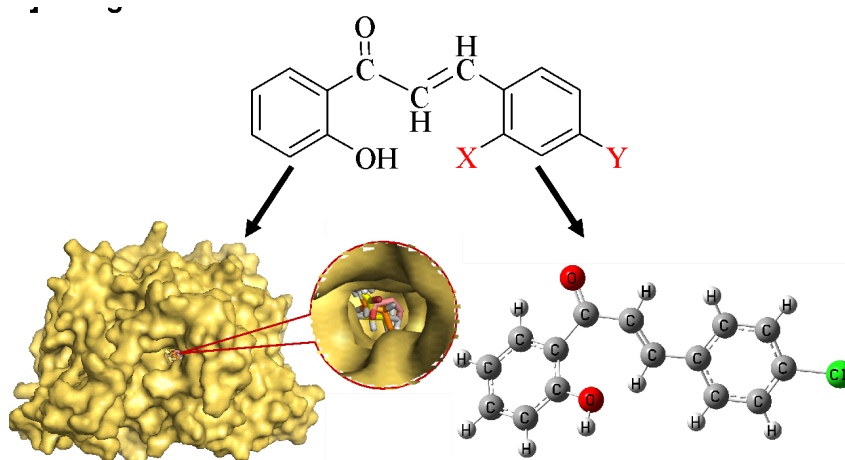
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Synthesis, Characterization of new 2'-hydroxychalcone derivatives and *in silico* prediction as potential SARS-CoV-2 inhibitor

Abstract

The microwave assisted synthesis of some new 2-hydroxychalcone derivatives and their characterization based on FT-IR, UV-Vis, ¹H-NMR, and mass spectra analysis have been described. Quantum chemical studies confirmed the structures of prepared chalcones. Results of molecular docking against SARS-CoV-2 (7BQY) main protease disclosed potential inhibition of prepared 2-hydroxychalcones than standard, hydroxychloroquine (HCQ) with the higher binding affinity. Molecular docking prediction has been validated by dynamics simulation. ADMET prediction suggested the non-carcinogenic and relatively safe properties than the standard. Hence, this study may be helpful to design a potent anti-COVID-19 candidate after therapeutic and pharmacological studies.





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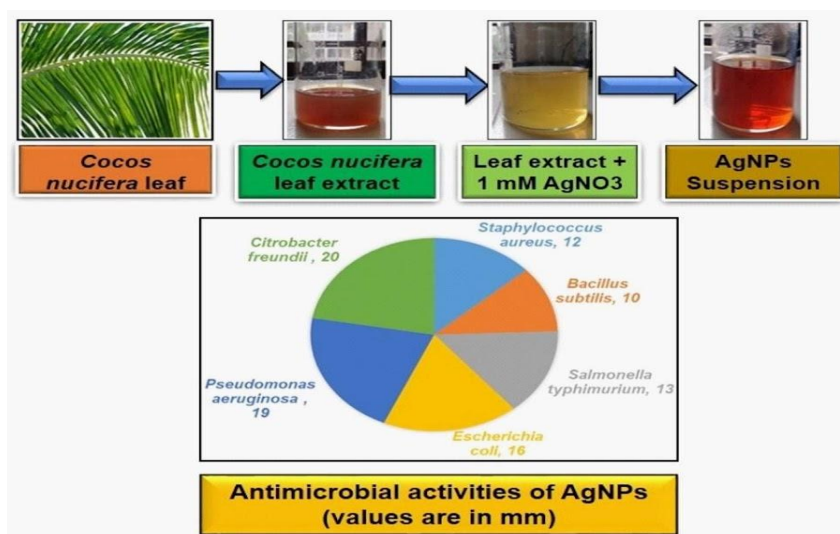
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Cocos nucifera leaf extract mediated green synthesis of silver nanoparticles for enhanced antibacterial activity

Abstract

In this work, we have reported green synthesized silver nanoparticles (AgNPs) with an average crystallite size of 14.2 nm that were fabricated by a newly developed technique for potential antimicrobial application induced by the importance of new antibiotics. The materials were successfully synthesized using *Cocos nucifera* leaf aqueous extract as the reducing and stabilizing agent and silver nitrate (AgNO_3) solution as a precursor. The synthesized material was characterized instrumentally by UV-visible (UV-Vis.) spectrophotometry, Fourier transform infrared (FT-IR) spectroscopy, scanning electron microscopy (SEM) and X-ray diffraction (XRD) analyses; and subsequently, their potential candidacy as antibacterial and antifungal agents against some common pathogens were evaluated. Antimicrobial potency of the synthesized AgNPs were tested by using the standard disc diffusion method and the results showed the zones of inhibition for both Gram-positive (*Staphylococcus aureus* and *Bacillus subtilis*) and Gram-negative (*Salmonella typhimurium*, *Escherichia coli*, *Pseudomonas aeruginosa* and *Citrobacter freundii*) bacteria were ranged from 10 to 20 mm. The NPs didn't show any inhibition against the two considered fungus viz. *Aspergillus niger* and *Tricoderma harzianum*. These results imply that the *Cocos nucifera* leaf extract mediated green synthesized AgNPs can be regarded as a potential candidate for antimicrobial application appreciably.





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In silico* study of arsenate reductase enzyme of *Bacillus megaterium

Abstract

Bacillus megaterium is a ubiquitous bacterial strain that produces the enzyme arsenate reductase that catalyzes arsenate(V) to more toxic arsenite(III). Due to the functional significance, present study was carried out to construct and validate the three dimensional (3D) structure of arsenate reductase of *B. megaterium* and study its interaction with arsenate. The 3D model was generated MODELLER using structure from *Bacillus subtilis* and *Staphylococcus aureus*. Superimposition of the model with the template structures were done by PyMOL. PATCHDOCK was used to perform molecular docking of the enzyme with arsenate ion and Fire Dock was used to refine the docked complexes. The highest geometric score containing docked complex was visualized and the intra-molecular interaction within it was evaluated by Discovery Studio. The sequence of *B. megaterium* arsenate reductase was characterized and its 3D structure was modeled appropriately so that the model can be useful for further study. The crucial amino acids were involved in binding to the arsenate ion in the docked complex were found to be Cys10, Thr11, Gly12, Asn13, Ser14, Cys15, His43 and Asp106. This study can be helpful in future to perform mutation in the active sites of the enzyme in order to inhibit the binding of arsenate ion.



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The binding mechanism of ivermectin and levosalbutamol with spike protein of SARS-CoV-2

Abstract

In this study, we have investigated the binding mechanism of two FDA-approved drugs (ivermectin and levosalbutamol) with the spike protein of SARS-CoV-2 using three different computational modeling techniques. Molecular docking results predict that ivermectin shows a large binding affinity for spike protein (- 9.0 kcal/mol) compared to levosalbutamol (- 4.1 kcal/mol). Ivermectin binds with LEU492, GLN493, GLY496, and TRY505 residues in the spike protein through hydrogen bonds and levosalbutamol binds with TYR453 and TYR505 residues. Using density functional theory (DFT) studies, we have calculated the binding energies between ivermectin and levosalbutamol with residues in spike protein which favor their binding are - 22.4 kcal/mol and - 21.08 kcal/mol, respectively. The natural bond orbital (NBO) charge analysis has been performed to estimate the amount of charge transfer that occurred by two drugs during interaction with residues. Molecular dynamics (MD) study confirms the stability of spike protein bound with ivermectin through RMSD and RMSF analyses. Three different computer modelling techniques reveal that ivermectin is more stable than levosalbutamol in the active site of spike protein where hACE2 binds. Therefore, ivermectin can be a suitable inhibitor for SARS-CoV-2 to enter into the human cell through hACE2.

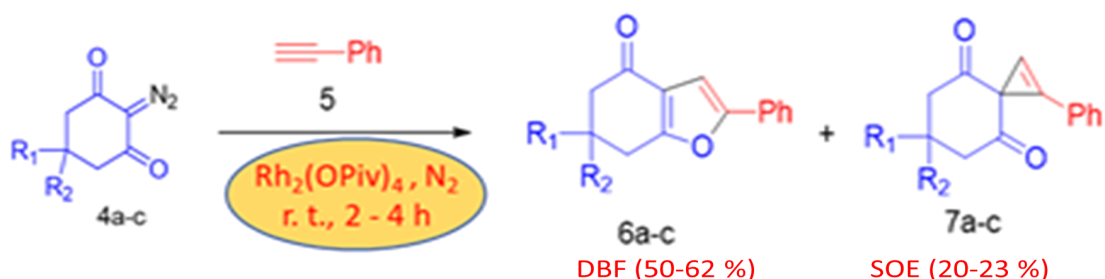


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DFT studies on electronic structure, thermochemistry, and reaction mechanism onto the synthesis of dihydrobenzofuran and spiro [2.5] oct-1-ene derivatives

Abstract

Dihydrobenzofuran and substituted furan derivatives exhibit biological activity and are present as structural skeleton in many natural products, medicinal agents, and industrially applicable compounds. This study represents a computational approach to explore the rhodium-catalyzed one-pot synthesis of dihydro benzofuran-4-one (DBF) and spiro [2.5] oct-1-ene (SOE) derivatives from 2-diazocyclohexane-1,3-dione, and phenylacetylene (PhA). Firstly, the B3LYP/GenECP/LanL2DZ/6-311++G (d, p) theoretical approach was applied to explore the mechanism of this reaction. The results indicate that a [3+2] cycloaddition reaction between diazo-compound and PhA proceeds through a two-step mechanism via a barrierless and highly exergonic process with relative free energy 73.61 kcal/mol to yield the kinetically-favored DBF derivatives. However, employing B3LYP and M06-2X levels of theory for the equilibrium geometry and thermochemistry calculation revealed that the cycloaddition reactions are spontaneous, and DBF is a thermodynamically more stable constitutional isomer SOE by 42.59 kcal/mol. Additionally, Merck molecular force field (MMFF94), followed by the B3LYP level of theory, was applied to predict the comparative stability for the several conformations of products, and Boltzmann weighted average ^1H chemical shift was computed by GIAO-B3LYP method. Finally, the UV-vis absorption was evaluated using time-dependent density functional theory (TD-DFT) for DBF and SOE.





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Preparation and characterization of Titanium dioxide (TiO₂), Ag-doped and Cr-doped TiO₂ nanoparticles

Abstract

Pure TiO₂, as well as Ag- and Cr-doped TiO₂ nanoparticles have been synthesized by the sol-gel method using titanium isopropoxide as the precursor of titania. The prepared nanoparticles were characterized by Scanning Electron Microscopy (SEM), Energy Dispersive X-ray Spectroscopy (EDS), X-ray Diffraction (XRD), and X-ray Photoelectron Spectroscopy (XPS). According to SEM images, all the samples were found to be of spherical crystal structures. Further, the XRD pattern exhibited their structures as of pure anatase form. From XRD data the average particle sizes were found to be 26.97 nm, 26.23 nm, and 24.33 nm for pure TiO₂, Ag-TiO₂, and Cr-TiO₂, respectively. The EDS spectra confirmed the presence of Ag, Ti, O, in Ag-TiO₂, and Cr, Ti, and O in Cr-doped TiO₂. The weight percentage of Ag, Ti, O were found to be 1.01%, 40.63%, and 58.37%, respectively in Ag-doped TiO₂, and that of Cr, Ti, and O in Cr-doped TiO₂ were 0.54%, 45.06%, and 54.40%, respectively. As investigated from the XPS analysis, in all of the samples titanium exists as Ti⁴⁺, silver as metallic Ag in Ag-TiO₂, and chromium as Cr³⁺ in Cr-TiO₂.



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The effects of oxidation states and spin states of chromium interaction with Sargassum Sp: A Spectroscopic and Density Functional Theoretical Study

Abstract

In this study, a systematic density functional theory (DFT) calculations were performed to study the interactions of transition metal chromium ion with different oxidation states and spin states and Sargassum sp. decorated with carboxylate(acetate) at the wB97XD/6-311++G(d,p) level of theory. Applying density functional theory (DFT), the structures and binding energies of chromium metal-carboxylate complexes at various oxidation states and spin states in gas phase were examined. The coordination strength of Cr(VI) with the acetate ligand was predominantly the strongest compare to the other oxidation states of chromium metal ions studied. Based on the calculated binding energies trend favors the tris $[\text{CrVI}(\text{AC})_3]^{3+}$ formation in the environment. Vibrational frequency analysis, for the homoleptic monomers of tris $[\text{CrIII}(\text{AC})_3]^0$ and $[\text{CrVI}(\text{AC})_3]^{3+}$ complexes, illustrate good harmony with the experimental and theoretical calculated frequencies. Using the time-dependent DFT (TD-DFT) at the level of CAM-B3LYP/6-311++G(d,p), the vertical excitation energies were obtained. The electronic transitions were recognized as the basis of HOMO-LUMO band gap energies. The stabilization energies derived using the second order perturbation theory, $E(2)$, of NBO analysis confirmed the greater charge transfer for the observed trends in the metal binding. The calculated value of interactions $\Sigma E(2)$ for $[\text{CrVI}(\text{AC})_3]^{3+}$ complex was higher compare to $[\text{CrIII}(\text{AC})_3]^0$ complex, which was according to energy analysis.

The findings of this study identify efficient electronic factors as major contributors to the metal binding affinities, with promising possibilities for the design of metal-ligand complexes and sensing of the metal ions.



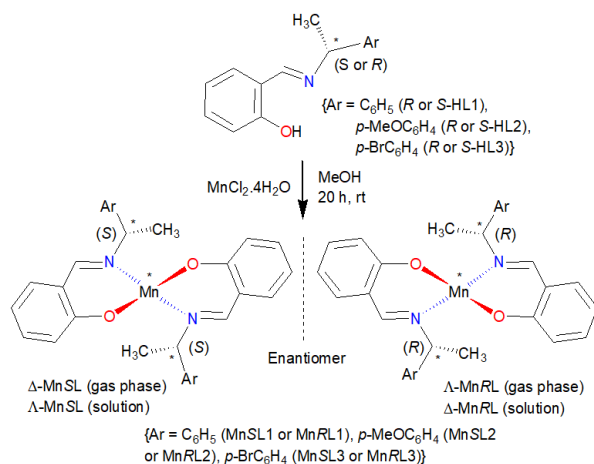
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Pseudotetrahedral *bis*[(*S* or *R*)-*N*-1-(*Ar*)ethyl-salicylaldiminato- κ^2 N,O]- Δ/Λ -Mn(II): Computational approach towards PXRD structural analyses

Abstract

The enantiopure Schiff bases (*S* or *R*)-*N*-1-(*Ar*)ethyl-salicylaldimine reacts with manganese(II) chloride to produce *bis*[(*S* or *R*)-*N*-1-(*Ar*)ethyl-salicylaldiminato- κ^2 N,O]-Mn(II) {*Ar* = C₆H₅ (MnSL₁ or MnRL₁), *p*-OMeC₆H₄ (MnSL₂ or MnRL₂) and *p*-BrC₆H₄ (MnSL₃ or MnRL₃)} with induction of Λ/Δ -chirality-at-metal (Scheme 1). The DFT optimized structures for diastereomeric pairs Λ -MnRL₁/ Δ -MnRL₁, Λ -MnRL₂/ Δ -MnRL₂, Λ -MnSL₂/ Δ -MnSL₂, Λ -MnRL₃/ Δ -MnRL₃ and Λ -MnSL₃/ Δ -MnSL₃ were calculated with the b3lyp functional and the basis set 6-31g(d), respectively. The experimental PXRD pattern for MnRL₃ was used for molecular structure determination using the Expo-2014 program followed by Rietveld refinement method. The PXRD structures were solved using the optimized structures for diastereomeric pair Δ -MnRL₃ and Λ -MnRL₃ as input files for calculations. The structure obtained from PXRD reveals that two molecules of N[^]O-chelates Schiff base ligands form a mononuclear, pseudotetrahedral N₂O₂-coordination sphere around the manganese atom. Both the PXRD structures and DFT calculations indicate a considerable distortion from the ideal tetrahedral to a pseudotetrahedral geometry around the metal atom. The results also suggest the possibility of mixture of both Δ -MnRL and Λ -MnRL diastereomers in the bulk sample. The excited state properties (UV-Vis. and ECD spectra) for the diastereomeric pairs Λ -MnRL₂/ Δ -MnRL₂ and Δ -MnSL₂/ Λ -MnSL₂ were calculated by TDDFT using b3lyp/def2svp//b3lyp/6-31g(d) level of theory. Comparisons of experimental and simulated ECD spectra suggest diastereomeric excess of Λ -MnSL or Δ -MnRL in solution resulting from diastereoselectively induced Λ - and Δ -chirality-at-metal.



Scheme 1. Syntheses of *bis*[(*S* or *R*)-*N*-1-(*Ar*)ethyl-salicylaldiminato- κ^2 N,O]- Λ/Δ -Mn(II) complexes.



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Homology modeling and molecular docking of a novel glycosylated analog of human erythropoietin

Abstract

Human erythropoietin (hEPO) regulates red blood cell production and is used in the treatment of anemia. The efficiency of the drug can be improved by increasing the carbohydrate content of hEPO. In this context, the objective of the present study was to generate a 3D model of hEPO analog with additional glycosylation and study its molecular interaction with the receptors. To insert an additional glycosylation site, the amino acid sequence of hEPO was modified at the position 132-134 to generate there a consensus motif N-X-S/T, which is essential for N-glycosylation. The prediction server, NetNGlyc, showed positive score for the newly created N-glycosylation site along with the three native sites of hEPO. The modified sequence was used to construct the 3D model of hEPO analog with the help of MODELLER. The good geometry of the analog's model was further confirmed by Ramachandran plot analysis which showed 92.5%, 6.1%, 1.4% and 0.0% of amino acid residues of the analog in the most favoured regions, additional allowed regions, generously allowed regions and disallowed regions, respectively. The model of the hEPO analog was then subjected to glycoengineering by GlyProt to attach the N-linked carbohydrate chains with it. The molecular docking of this glycosylated hEPO analog with the EPO-receptors was performed by ZDOCK. The docking study showed that the hEPO analog with the additional glycosylation had better docking score (2243.492) in comparison to the native hEPO (2065.279). Thus the computational modeling and docking study indicated that the glycosylated hEPO analog has significant potential which should be considered for further analysis to get improved drug efficacy.



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Interaction of different conducting organic polymers (COPs) towards cyanogen halides as gas sensors: density function theory (DFT) study.

Abstract

Density functional theory (DFT) studies have been carried out to evaluate the ability of conducting organic polymers (COPs) as gas sensors for cyanogen halides (XCN, where X=Br, Cl and F). In this study, geometry optimization, binding energy calculations, charge analysis, HOMO–LUMO orbital analysis, and UV–vis spectra have been performed at M06-2x/6-31+G(d,p) level of theory. The large binding energies have been found for PANI-CN_X complexes. But four COPs bind with CNBr with larger binding energies than the rest two analytes, CNCl and CNF. The binding energies are -14.30, -11.22, -12.49, -14.56 kcal/mol for PEDOT-CNBr, PTh-CNBr, PPY-CNBr and PANI-CNBr, respectively. It is found that the binding energy increases with increasing the atomic number of halogens in XCN (X=Br, Cl, and F). NBO, HOMO, LUMO and uv-vis data also support the fact that four COPs (PEDOT, PTh, PPY and PANI) show more sensitivity towards CNBr than CNCl and CNF. But among four COPs, PEDOT and PTh will be suitable candidates to sense CNBr as gas sensors.



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A review of ZnO nanoparticles against SARS-CoV-2 virus and other viral infection with computational study

Abstract

Tiny particles containing genetic material (DNA/RNA) and surrounded by protein coat are called viruses. Some viruses can protect host against other infections some are pathogenic including common cold, influenza, chickenpox, human immunodeficiency virus (HIV), SARS-CoV-2 and others. A proliferation of a pathogenic virus inside host cell is called viral infection. This study describing a review about the applications of ZnO nanoparticles for the treatment of viral infections including global pandemic rising virus SARS-CoV-2 (COVID-19) and molecular docking study also optimised. There are various methods available for synthesizing nanoparticles including physical, chemical, and biological. Biological method involving nanoparticles synthesis by using plant extract of any part or any microorganism extract. This biological method is environmentally friendly process and referred as safe than physical and chemical methods for producing toxic chemical as byproducts.

International Conference on Materials Science & Computation (ICMSC-21)

Time: At 12:00 on 21 August 2021

Venue: WMSRC, Jahangirnagar University, Dhaka, Bangladesh

Organizing committee:

Convener: Professor Dr. Mohammed Enamullah, Department of Chemistry, JU.

Co-convener: (1): Professor Dr. Mohammad Shahedur Rahman, Department of Biotechnology & Genetic Engineering, JU, (2) Professor Dr. Abdus Salam, Department of Chemistry, DU, Dhaka.

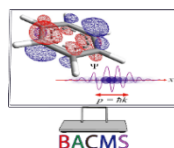
Secretary: Professor Dr. M Mosharef Hossen Bhuiyan, Department of Chemistry, CU, Chittagong.

Joint Secretary: Mohammad Khairul Islam, WMSRC, Jahangirnagar University, Dhaka.

Treasurer: Professor Dr. Royhan Uddin, CoU, Comillah, Email: royhanbau@yahoo.com

Sub-committee:

- (1) **Invitation:** Prof. Dr. M. Enamullah, Professor, Dr. Al-Nakib Chowdhury, Prof. Dr. Mossharaf Hossain, Professor Dr. Imdadul Islam, Prof. Dr. Mohammad Shahedur Rahman, Prof. Dr. Abdus Salam.
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- (3) **Publication:** (i) Dr. Joyanta Kumar Saha, Associate Professor, Depart. Chem., JnU, Dhaka; (ii) Mortuza Mamun, Dept. Chem., JU, (iii) Siam Abdullah, Department of Chemistry, JU, (iv) Tarek Aziz, Department of Chemistry, JU, (v) Shirazum Munira, Depart. Chem., JnU, Dhaka. (vi) Afsana Mim, Dept. Chem., JU.
- (4) **Communication (Electronics):** Professor Dr. Imdadul Islam, Department of Computer Science & Engineering, JU; (ii) Md. Khairul Islam, Dept. Chem., JU, (iii) Tarek Aziz; Dept. Chem., JU. (iv) Abdullah Hira, Dept. Chem., JU, (v) Habiba Afrin Liza, Dept. Chem., JU
- (5) **Press & publicity:** (i) Md. Mazharol Hoque, Associate Professor, Dhaka City College, Dhaka, (ii) Ms. Naima Thahsin, Department of Biotechnology & Genetic Engineering, JU, (iii) Tazrin Islam Tonny, Dept. Chem., JU, (iv) Amina Khan Resma, Dept. Chem., JU, (v) Fazle Elahi Munna, Dept. Chem., JU.



Bangladesh Association for Computational Materials Science (BACMS)

International Conference on Materials Science and Computation

Inaugural Session
08.00 PM, 20 August 2021



Scientific Session
12.00 PM, 21 August 2021

WMSRC, Jahangirnagar University, Dhaka, Bangladesh

Guests & Speakers



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York University
Toronto, Canada



Prof. C. Janiak
Heinrich-Heine-University
Düsseldorf, Germany



Prof. Wen-Hua Sun
Chinese Academy of Science
Beijing, China



Prof. W. Linert
Vienna University of Technology
Vienna, Austria



Prof. W. A. Houry
University of Toronto
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Prof. J. Müller
Westfälische Wilhelms-Universität
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Prof. Tooru Tanaka
Saga University
Saga, Japan



Asso. Prof. D. E. Herbert
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Senior Scientist, CAES, DU
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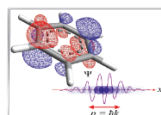
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