



## Contents

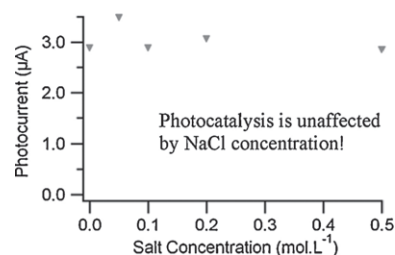
### Articles

**Robin Brimblecombe, Jun Chen, Pawel Wagner, Timothy Buchhorn, G. Charles Dismukes, Leone Spiccia, Gerhard F. Swiegers**

► A *PSII*-WOC model complex photocatalyzes O<sub>2</sub> formation in non-potable and seawater. ► No Cl<sub>2</sub> is observed under illumination at 1.20 V (vs. SHE). ► Effect comparable to the *PSII*-WOC in aquatic organisms (operate at 1.25 V vs. SHE).

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Photocatalytic oxygen evolution from non-potable water by a bioinspired molecular water oxidation catalyst

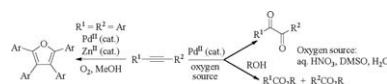


**Jacques Muzart**

► This review highlights the Pd-catalyzed procedures leading to the oxidation of C=C bonds. ► The procedures are exemplified using 19 equations and 8 tables. ► Plausible mechanisms and reactive intermediates are depicted in 5 schemes.

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Pd-catalyzed oxidation of alkynes

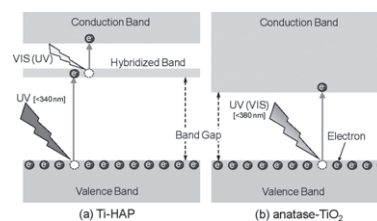


**Mineharu Tsukada, Masato Wakamura, Naoya Yoshida, Toshiya Watanabe**

► Ti substitution in hydroxyapatite (HAP) formed hybridized state in HAP band gap. ► Hybridized state caused absorption-edge lowering of Ti-substituted HAP (Ti-HAP). ► Ti position in Ti-HAP was predicted to be columnar, Ca(1), site. ► Photocatalytic model of Ti-HAP was proposed to be a two-step excitation model. ► Acetaldehyde gas decomposition by Ti-HAP using UV was enhanced by adding VIS.

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Band gap and photocatalytic properties of Ti-substituted hydroxyapatite: Comparison with anatase-TiO<sub>2</sub>

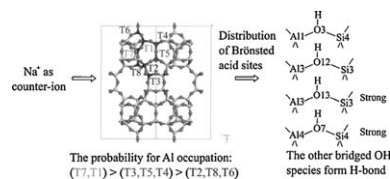


**Yan Li, Wenping Guo, Weibin Fan, Shuping Yuan, Junfen Li, Jianguo Wang, Haijun Jiao, Takashi Tatsumi**

*Journal of Molecular Catalysis A: Chemical* 338 (2011) 24

A DFT study on the distributions of Al and Brønsted acid sites in zeolite MCM-22

► Framework Al distribution in MCM-22 was studied with Na<sup>+</sup> as counter-cation. ► The most probable sites for locating Al are T7 and T1, while T2, T8 and T6 are much less stable. ► Both isolated and H-bonded Si–OH–Al species were contained in H-MCM-22. The calculated OH frequencies agree well with the experimentally observed values. ► Al3–O13H–Si3 and Al4–O7H–Si4 show stronger acidity than Al1–O3H–Si4 and Al3–O12H–Si3.

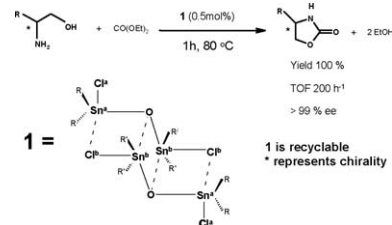


**Sharon Pulla, Vineed Unnikrishnan, Punnamchandaram Ramidi, Shane Z. Sullivan, Anindya Ghosh, Jerry L. Dallas, Pradip Munshi**

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Interaction of substrate and catalyst during the formation of oxazolidinones from 2-aminoalcohols and diethyl carbonate using recyclable 1,3-dichlorodistannoxanes

► Synthesis and mechanism of oxazolidinone from 2-aminoalcohol and diethyl carbonate. ► Tetrachlorodistannoxane catalyst, [(RR'<sup>2</sup>SnCl)<sub>2</sub>O]<sub>2</sub>, used is severally recyclable. ► Reaction completes in 1 h at 80 °C with 100% yield and >99% ee. ► Turn over frequency of 200 h<sup>-1</sup> is much higher than the reported value of 4 h<sup>-1</sup>.

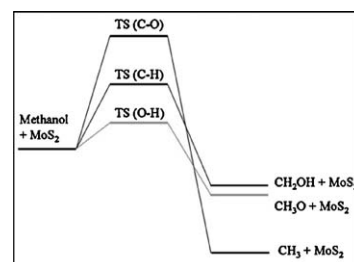


**Yan-Yan Chen, Mei Dong, Zhangfeng Qin, Xiao-Dong Wen, Weibin Fan, Jianguo Wang**

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A DFT study on the adsorption and dissociation of methanol over MoS<sub>2</sub> surface

► Adsorption and dissociation of methanol on MoS<sub>2</sub> surface were investigated by DFT. ► Methanol molecule prefers being adsorbed through its oxygen atom on the corner sites. ► O–H bond scission is the most favorable pathway for methanol dissociation. ► CH<sub>3</sub>O is the dominant surface species upon the exposure of methanol on MoS<sub>2</sub>.

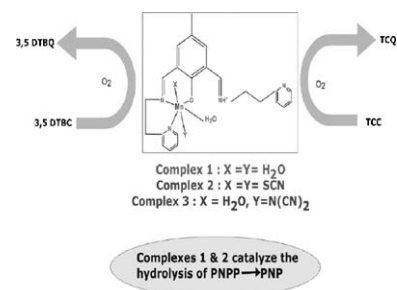


**Averi Guha, Kazi Sabnam Banu, Arpita Banerjee, Totan Ghosh, Santanu Bhattacharya, Ennio Zangrando, Debasis Das**

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Bio-relevant manganese(II) compartmental ligand complexes: Syntheses, crystal structures and studies of catalytic activities

► Syntheses, characterisation and catalytic efficiency of three new Mn<sup>II</sup> complexes. ► In spite of the ligand being dinucleating the complexes were mononuclear. ► Catecholase and phosphatase activities shown by mononuclear Mn<sup>II</sup> complexes. ► Protonation of one imine N results in unusual nuclearity and catalytic efficiencies.



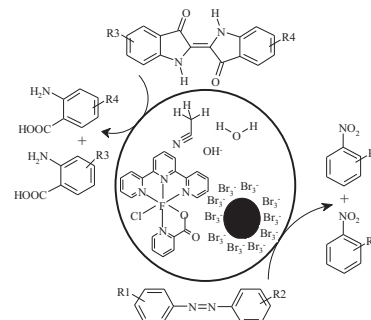


**Rajenahally V. Jagadeesh, T. Kiran,  
Pundlik R. Bhagat, S. Senthil Kumar,  
P. Nithya, F. Nawaz Khan, A. Sivakumar**

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Design and mechanism of iron catalyzed carbon-carbon bond cleavage and N-oxidation processes of hazardous dyes for selective synthesis of nitroarenes and aminoarene-carboxylic acids

►Iron Catalyzed oxidative-degradation process has been developed for the selective conversion of environmentally hazardous azo and indigo dyes into nitrobenzenes and anthranilic acids respectively. ►The catalytic process involves the selective oxidative degradation of -N=N- and -C=C- bonds of azo and indigo dyes respectively. ►A common oxidative degradation mechanism which operates in both the dyes has been proposed and an identical related kinetic model was designed.

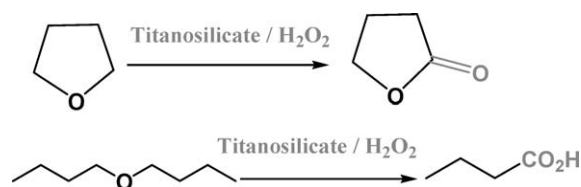


**Manickam Sasidharan, Asim Bhaumik**

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Catalytic oxidation of cyclic ethers to lactones over various titanosilicates

►Catalytic oxidation over TS-1, TS-2, Ti- $\beta$ , Ti-MCM-22, VS-1, CrS-1, CrS-2. ►Partial oxidation of cyclic and open-chain ethers. ►Synthesis of lactones from ethers. ►Titanosilicates vis-à-vis other metasilicates.

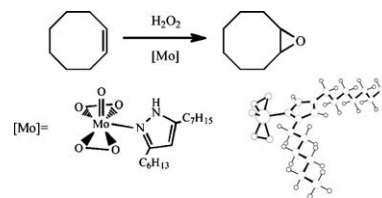


**Matthew Herbert, Francisco Montilla,  
Agustín Galindo**

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Olefin epoxidation in solventless conditions and apolar media catalysed by specialised oxodiperoxomolybdenum complexes

►Solubility enhancements from functionalised ligands facilitate catalytic activity. ►Pyrazole complexes show higher activities than bipyridine analogues. ►3-Hexyl-5-heptylpyrazole gave the highest activity under solventless conditions.



**Juan F. Miñambres, María A. Aramendía,  
Alberto Marinas, José M. Marinas,  
Francisco J. Urbano**

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Liquid and gas-phase Meerwein-Ponndorf-Verley reduction of crotonaldehyde on ZrO<sub>2</sub> catalysts modified with Al<sub>2</sub>O<sub>3</sub>, Ga<sub>2</sub>O<sub>3</sub> and In<sub>2</sub>O<sub>3</sub>

►Al, Ga or In impregnated ZrO<sub>2</sub> catalysts showed Lewis acidity. ►Coprecipitated counterparts are more basic and Lewis component is lacking. ►Impregnated catalysts were the most active in selective crotonaldehyde reduction ►High selectivity (80–88%) to crotyl alcohol was found for all catalysts at 200 °C.

