Characterization of Pyrite Particles by Molecular Modeling Methods

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Pyrite is the most abundant of metal sulfides in nature; Pyrite is often considered as an unwanted substrate in graphite industry. The quality of the nation's graphite resource is often degraded due to intimate association of this mineral. The data generated in this research will pave an initial step in suggesting an innovative of way of purifying graphite and adding a value for hither todate unwanted mineral pyrite. Pyrite showed great promise as a starting material for decontamination of water polluted with organic pollutants in both the presence and absence of light .It is an intrinsic semiconductor that exhibits both n- and p-type conductivity. The band gap is around 1 eV thus it can efficiently be used as a photo catalyst in the destruction of both organic and inorganic pollutants. Also an understanding of its reactivity is important for such applications as ore processing by flotation and solar energy conversion, as well as for geochemical processes like the production of acid mine waste waters. All of these processes involve reactions at pyrite surfaces and it is consequently important to understand the nature of these surface reactions. Pyrite surface chemistry plays an important role in many natural and technological systems, for example in extractive metallurgy, coal processing, geochemistry, acid-mine drainage and pollution control. Numerous studies on the nature of pyrite surface reactions have been conducted using various methods. The research is devoted to the development of theoretical cluster model for pyrite to mimic its properties in solid state. The data validation was made with IR spectroscopic data. For this pyrite clusters were developed with increasing complexity. The Gaussian 03 code was used to conduct calculations for geometry optimizations, frequency calculations and single point energy calculations using *abinitio* HF method. All clusters were successfully optimized at 3-21G level. The experimental IR data showed poor resemble with the calculations at 3-21G level. In order to validate the model calculations of pyrite clusters with 12, 22 and 84 atoms are currently in progress.

Key words: *Pyrite, HF method, Abinitio*