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Organic inhibitors of corrosion of metals: quantum chemical study

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LAP Lambert Academic Publishing Jun 2013, 2013. Taschenbuch. Book Condition: Neu. 220x150x5 mm. This item is printed on demand - Print on Demand Neuware - Results of quantum chemical computations of molecules of organic inhibitors (OIn) of corrosion and hydrogen absorption by metals of 9 different series, for some of groups - also adsorbed on clusters modeling Al and Cd surface in various oxidation states (the model substrates contained up to 25 atoms of metal and O, H - in case of hydroxides) were compared to experimental data on efficiencies of protective action (EPA) against corrosion of metals. Energies of boundary orbitals (HOMO, LUMO) and dipole moments of isolated molecules of OIn as well as changes of atomic charges on OIn atoms when OIn molecule adsorbed have been computed using semi-empiric MNDO quantum chemistry method. Found correlations between EPA and changes of electric charge on heteroatoms (as N, O.), also change in value of dipole moment and in total molecular charge due to adsorption of OIn on the metal surface were most significant. Data on efficiencies against hydrogen absorption by steel were compared to data obtained from quantum chemistry for individual molecules. The material put together in this book is...



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