Patent No. 3702339

Program and Related Device Based on Conductor Model for Analyzing Molecules and Other Particles Adsorbed on Metal Surfaces

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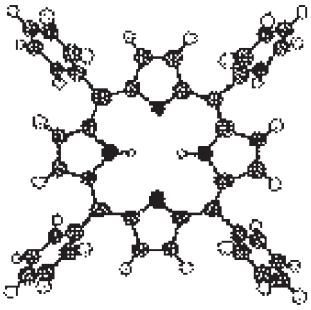
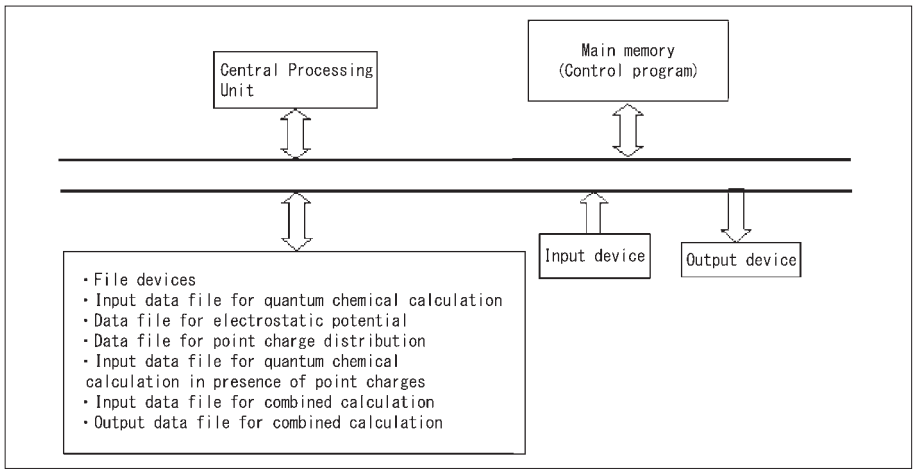


Molecular model

Overview of technology

This invention provides a method of numerical analysis that is more rational and more applicable than conventional methods. To summarize, the invention solves problems in conventional methods and provides a more rational, accurate, and applicable method of computer analysis for clarifying characteristic values and stable structures of molecules or clusters of molecules adsorbed on metal surfaces. Specifically, when evaluating the interactions induced between the adsorbed molecules and the metal surface, this method treats the metal as a conductor and approximates the charges induced on the surface of the conductor by the adsorbates as a collection of point charges, each situated within each microscopic region dividing the conductor surface. By combining quantum chemical calculation in the presence of the determined point charges and calculation of the empirical inter-atomic potential function expressing the repulsive and the dispersion interactions,



Configuration diagram

the invention enables practical evaluation of various characteristic values and the stable structure of a molecule or a cluster of molecules adsorbed on the metal surface. Accordingly, this invention enables analysis of molecules and other particles adsorbed on rough surfaces, a difficult task using conventional methods; moreover, it can provide more accurate results for characteristic values and structural stability for molecules and other particles adsorbed on flat metal surfaces.

Molecular simulation analysis

Molecular simulation analysis is a field of computational chemistry. This means of analysis is now attracting attention in light of problems arising in chemistry involving complex systems, many of which problems cannot be solved without the aid of computers (Fig. 1). Recent advances in the processing capacity of computers have greatly increased the importance of molecular simulation analysis, which is now considered as a third research method alongside experimentation and theory. Numerical calculations on computers based on the molecular orbital (MO) method or the molecular dynamic (MD) method can predict reactions, syntheses, and interactions between molecules and compounds. Well known examples of molecular simulation analysis include prediction of the dielectric constant of an LSI, molecular design of drugs, and in-silico screening by computers including docking tests for drug candidate substances and specific proteins.

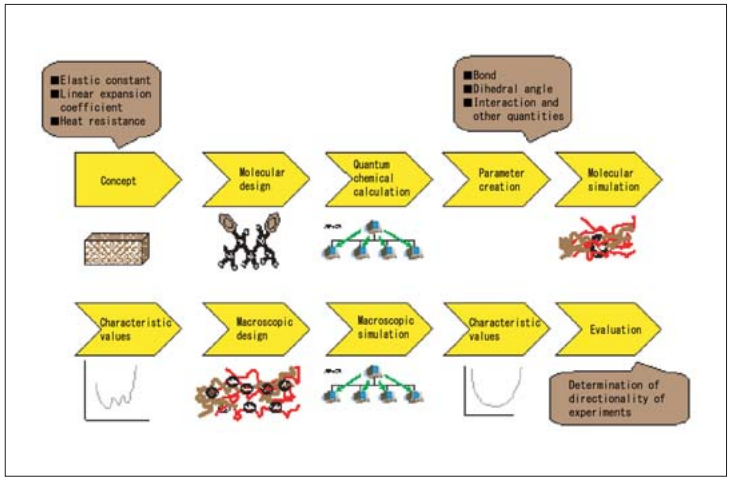
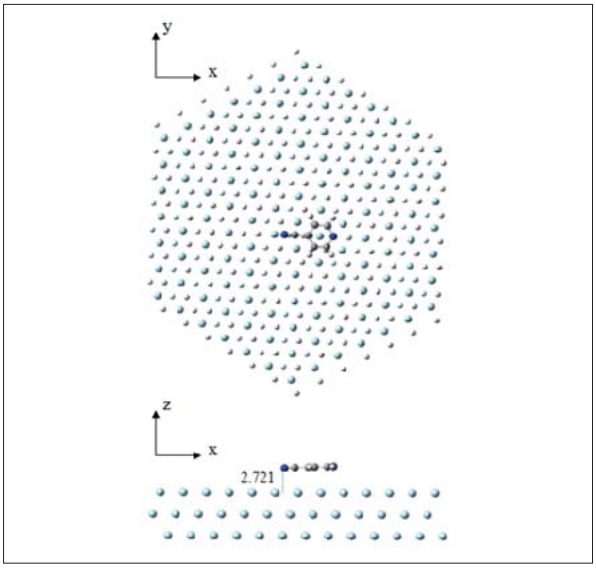


Fig. 1 : Flow chart of analysis



Example of structural calculation for a molecule adsorbed on a metal surface. The figure shows the stable structure of a benzonitrile molecule (center in the upper figure) adsorbed on an Au (111) surface (the many pale blue spheres represent gold atoms). he calculated distance between the gold surface and the benzonitrile molecule is 2.721 angstroms (center in the lower figure).

Fig. 2 : Example calculation result

Among diverse simulation analyses, this patent concerns a technology related to surface chemistry that tests and researches the conductivity and stability of substances when molecules are adsorbed on a surface. This technology is used in manufacturing nanodevices and MEMS and for studying the behavior (local structures and electronic states) of molecules on solid surfaces such as metal surfaces. The chemical reactions on solid surfaces differ from those in liquids, and are attracting particular attention in recent chemical research. This patent is executed as a numerical calculation in the form of an algorithm of a computer program (Fig. 2).

Commercial production

This patent is licensed to Simulatio Corporation together with similar inventions and the program. Simulatio Corporation provides it as entrusted simulation analysis services.

(Article written by SAWADA Fumitake, Expert, Intellectual Property Management Group, Research Promotion Department)

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