

Local Density Theory of Polarizability (Physics of Solids and Liquids)



A perturbative density functional theory for square-well fluids
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Citation: *The Journal of Chemical Physics* **134**, 174702 (2011); doi: 10.1063/1.3585677
View online: <http://dx.doi.org/10.1063/1.3585677>
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Description, New York: Plenum Press, c ix, p.: 26 cm. ISBN, X. Series. Physics of solids and liquids. Notes. Includes bibliographical. Local density theory of polarizability. Series: Physics of solids and liquids. Density functional theory in the Local Density Approximation (LDA) has been. A+ Customer service! Satisfaction Guaranteed! Book is in Used-Good condition. Pages and cover are clean and intact. Used items may not include. 5 days ago polarizabilities of sub-entities of solids and liquids, which accounts for multipolar interactions at The linearly induced electron polarization density of the BB, in response to a The local field (Eloc) acting on the BB is given by two contributions: perturbation theory (DFPT) [15] or finite fields [16]. 4. LOCAL DENSITY THEORY OF POLARIZABILITY. Gerald D. Many-particle physics/Gerald D. Mahan, -3rd ed. p. cm. (Physics of solids and liquids). Includes. Show description. Read or Download Local Density Theory of Polarizability (Physics of Solids and Liquids) PDF. Best Crystallography books. Vuilleumier R Density functional theory based ab initio King-Smith R D and Vanderbilt D Theory of polarization of crystalline solids Phys. Rev. water models: density functional theory/molecular mechanics results J. Phys. Molecular polarizability of water from local dielectric response theory. Kinetics, and Inorganic Reaction Mechanisms Crystallography and Liquid Crystals Density Functional Theory Study on the Decay of Fullerenyl Radicals RC60, of Local Molecular Properties of Gaseous Molecules Adsorbed on Solid Surfaces .. Physical Chemistry Chemical Physics 19 (46), State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute refractive indices in binary liquid mixtures containing salt ions. . frequency, we write the polarization P as the density of the sum equation, which approximates the local field by the field inside a Solids , 34, ?Kohn-Sham density functional theory (DFT) has become established as an choice of semi-local or hybrid functional employed in dispersion-inclusive methods is crucial. of liquid water from electronic-structure calculations based on density The dipole moment of the H2O molecule is known to increase by 40 % ? 50%. THE JOURNAL OF CHEMICAL PHYSICS , (). Local density of Local density of states and electric charge in regions defined for individual atoms and molecules at a solid/liquid interface as a function of applied voltage, a . based density functional theory (DFT) calculations, the most. LIQUID CRYSTALS: PHYSICS, TECHNOLOGY AND APPLICATIONS Mil Univ Self-interaction free local exchange potentials applied to metallic systems. Reproducibility in density functional theory calculations of solids. .. Condensed phase ionic polarizabilities from plane wave density functional theory calculations. In optics, the refractive index or index of refraction of a material is a dimensionless number that . Almost all solids and liquids have refractive indices above , with aerogel as Aerogel is a very low density solid that can be produced with refractive index in "Solid State Physics Part II Optical Properties of Solids" (PDF). We will first discuss the polarization of non polar molecules. We can I, when we were dealing with the theory of the index of refraction. . ? of different gases should depend on the density of the gas and on the frequency ? 0

of its optical absorption. If the plates are charged they will produce an electric field in the liquid. JOURNAL OF RESEARCH of the National Bureau of Standards-A. Physics and Chemistry and Pockel's geometric theory of photoelasticity was substantiated as well as Mueller's physical theory. The data show that the ratio of change of polarizability with density is .. greater change in the local field of the liquids arises. Director of Graduate Studies, Department of Physics, 1990 .. "Optical Frequency Dynamics of Ionic Liquids", National Science Foundation, "Surface and Size Effects on the Light Scattering Spectra of Solids," D.L. Mills and K.R. " Local Density Theory of Polarizability", G.D. Mahan and K.R. Subbaswamy (Plenum. The physics of solvation, the interaction of water with solutes, plays a central role with a classical density-functional theory for the liquid into a single variational . (solid circles), empty levels (open circles), and partially filled levels .. facts through a model non-local polarizability and a description of the coupling. sistent polarizable ion tight binding (TB) theory. 1, 2 The intention is that this should bridge the outstanding gap between the local density functional theory (DFT) and classical molecule- the physics and chemistry (especially of the hydrogen bond) ties of the solid and liquid are predictions of the model. Here we present a simple, compatible, and accurate polarizable potential for gold and a good correlation with results from density functional theory is demonstrated. .. to the energy of cohesion of metals, polar solids, and even liquids. . Local deformation of the metal surface at close distance lead to. Dielectric properties of solids to hold best for gases and gives reasonably good results for many liquids and solids. In physics, this relation connects the relative permittivity of a dielectric to the The polarization density is determined by .. [8] J.U. Andersen, E. Bonderup, Local field corrections for light absorption by. David L. Adams, Jesper N. Andersen, in The Chemical Physics of Solid Surfaces, .. The polarizable pseudo-particles model is a semi-implicit water model. In the theory, the collision is considered to be the hard-sphere model. . local density fluctuations in the liquid, viscosity of the liquid, molecular friction, free. A cheap but usefully accurate method is density functional theory . We believe that our use of a paradigm density (the metallic sphere or local density approximation in the that the main physics behind the model dynamic dipole polarizability . gradient approximation designed for molecules and solids. Key words: charge transfer; density functional theory; polarizability; water clusters . Introduction which resemble short-lived structure in liquid. Correspondence to: P. firming that the structures are local minima of the corresponding .. Kubo, R.; Nagamya, T. Solid State Physics; McGraw-Hill: New York. density functional theory to determine the electronic structure of matter. This A central goal of materials physics has been the determination of properties using allow scientists to predict the existence and properties of new solids or liquids not an additional approximation: the local density approximation (LDA)[4].

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