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The theoretical calculation at the RI-CC2/TZVPP//DFT-D2-B97-D/TZVP level nicely reproduced the experimental CD spectra in both excitation energy and rotational strength without any shift or scaling. These calculations afforded the electric and the magnetic transition dipole moment vectors in [n]helicenes, allowing us to discuss the observed rotational strengths as a function of the number of benzene rings.

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This theoretical study reveals that the direct Si-ligand dissociation by NIR light is difficult to activate because of the high dissociation energy even in excited states, i. e., >1.30 eV. Instead, irradiation generates the IR700 radical anion, leading to acid-base reactions with nearby water molecules (i. e., calculated pK_b for the radical anion is 7.7) to produce hydrophobic ligand ...

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The experimental method is a convincing and intuitive means to investigate the energy absorption capacity of such structure , , , and can provide the baseline data for validating and deriving material parametric values for numerical and theoretical studies [10,13,14,24]. However, depending on the scope of an experimental program, the tests can be expensive and time-consuming.

~~Numerical, theoretical, and experimental studies on the ...~~

Theoretical and experimental studies on J_c and AC losses of 2G HTS coils Weijia Yuan, M D Ainslie, W Xian, Z Hong, Y Chen, Y Yan, R Pei, T A Coombs Department of Electronic & Electrical Engineering

~~Theoretical and experimental studies on J_c and AC losses ...~~

This Ciba Foundation international symposium in 1992, which I proposed to the foundation in 1991, gathered together 25 of the most prominent philosophers and scientists working on consciousness at that time. What is particularly interesting about

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We report the theoretical and experimental study of calibration-free heterodyne phase-sensitive dispersion spectroscopy (HPSDS) in the mid-infrared using a direct current modulated mid-infrared quantum cascade laser (QCL). The modulation of QCL current at several hundred MHz or higher generates the synchronous frequency and intensity modulation of the QCL emission.

~~Theoretical and Experimental Study of Heterodyne Phase ...~~

The influence of different substituents in imidazolium ILs and urea addition were analyzed using experimental measurement and theoretical molecular calculations. Physicochemical properties of neat ILs and IL-Urea solutions, including density, viscosity, conductivity, thermogravimetric analysis (TGA), and solvatochromic parameters (β value and π^* value), were thoroughly investigated.

~~Theoretical and experimental studies of ionic liquid-urea ...~~

Theoretical physics is a branch of physics that employs mathematical models and abstractions of physical objects and systems to rationalize, explain and predict natural phenomena. This is in contrast to experimental physics, which uses experimental tools to probe these phenomena. The advancement of science generally depends on the interplay between experimental studies and theory.

~~Theoretical physics - Wikipedia~~

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This study conducts an experimental and theoretical investigation of the influence of a polyvinylpyrrolidone (PVP) capping layer on silver nanowire (AgNWs) networks. Through a washing method, a PVP layer on AgNWs was removed and the contact resistance (R_C) between AgNWs was reduced, thereby obtaining a reduced sheet resistance (R_S) of AgNW film. During the washing process, the thickness of the PVP layer decreased to 1 nm with an increasing number of washes, as demonstrated by a molecular ...

~~Influence of polyvinylpyrrolidone (PVP) capping layer on ...~~

So what's the big difference between theoretical and experimental probabilities? The main difference is that a theoretical probability is calculated based only on the knowledge of the situation.

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Both the theoretical and experimental results indicated that the pressure field shifted towards the narrow side. As the central height h_c increased, the overall amplitude of the pressure field decreased; this indicates that the pressure field of the inclined airflow film is sensitive to changes in h_c with a small gap height.

~~Theoretical modeling and experimental study of pressure ...~~

Theoretical and experimental study on the thermally dependent transient response of the high power continuous wave Yb-doped fiber laser. Mingjian Yan, Siyu Li, Zhigang Han, Hua Shen, and Rihong Zhu. Appl. Opt. 58(20) 5525-5532 (2019) Suppression of inter-modal four-wave mixing in high-power fiber lasers.

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Theoretical and Experimental Studies of an S-Catamaran

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Theoretical and Experimental. ... implicit) analysis step was used in this study for the single-layer. and multilayer cylindrical structures with optional geometric non-linearity.

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Theoretical and Experimental Studies. ROBE R T JANSSON. Doctoral Thesis in

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Concrete Structures. Stockholm, Sweden 2013. www.kth.se. TRIT A-BKN. Bulletin 117, 2013. ISSN 1103-4270. ISRN KTH/BKN/B ...

~~Fire Spalling of Concrete: Theoretical and Experimental ...~~

Comprehensive Photophysical Properties of Thiophene/Phenylene Co-oligomers Investigated by Theoretical and Experimental Studies Jie Kong Beijing National Laboratory for Molecular Sciences (BNLMS), Key Laboratory of Photochemistry, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, People's Republic of China

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