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Accepted Abstracts

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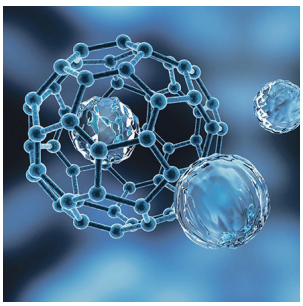

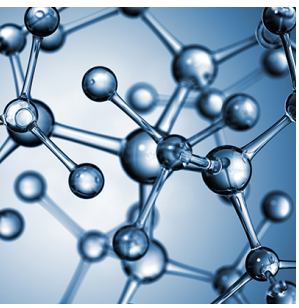
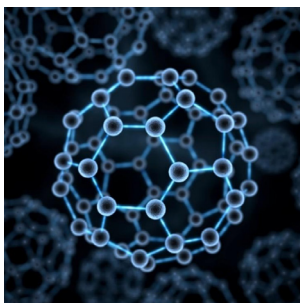


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Finite range interaction Gaussian as a probe for harmonically trapped Bose gas in effective quasi-two dimensions

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A system of harmonically trapped N=16 spin-0 bosons in quasi-2D symmetrical x-y plane interacting repulsively via a finite range Gaussian potential is studied under an externally impressed rotation about the stiffer z-axis. The exact diagonalization of N-body Hamiltonian matrix in each subspace of quantized total angular momentum 0<L<4N is performed beyond the Lowest Landau level approximation [1]. We considered the interaction-range parameter σ =0.30, 0.50 and 0.75 to study the finite-range effects on the many-body ground state of the rotating system. It is observed that with increase in interaction range σ, the quantum mechanical coherence extends over more and more particles within the system size resulting in an enhanced stability of the ith vortical state with angular momentum L(Ωci) leading to a delayed onset of the next vortical state L(Ωc(I+1)) w.r.t rotational angular velocity. For a given vortical state, there is an increase in the critical angular velocity L(Ωci) with increasing σ. There is decrease in length of plateaus with increasing σ in stability line. We observed that more number of stable micro-plateaus evolved with increases in the interaction range σ. We also observed that the nucleation of vortical states is independent of interaction range σ. With increase in σ, there is no notable change in von-Neumann entropy (S1) [2] and the degree of condensation (Cd) in the slow-rotating regime 0< L< N; however, for moderately rotating regime with L< 2N, the significant variation in S1 and Cd are observed [3]. Quantitatively, the degree of condensation increases and von-Neumann entropy decreases for increasing σ. We also have observed that there is cross-over in von-Neumann entropy S1 (degree of condensation Cd) over interaction range σ for given angular momentum L-state. We also plot iso-surface density plots for conditional probability to study the nucleation of vortex states. Which is one of the signatures of rotating Bose gas, we report that with the increase in interaction range σ, the probability density starts accumulation at the edge of vortices and p=2-fold diagonally symmetric state emerged into singly quantized vortical state for the system size [4]. We also noticed that the vortical state entry in the Bose-gas condensate is favored by the higher σ. It is found that the finite-range effect has more impact on the unstable states as compared to stable states for given set of parameters. Subsequently, the breaking of rotational symmetry of the system in the unstable L-states is observed and this effect becomes more prominent at larger values of σ.

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Fine-tuning the strategy XtalOpt + Gibbs2 codes. Application to thermoelectric compounds (AgCl, PbTe and CoSb3) under stress: Phase diagrams pT

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The ultimate objective of this work is the proposal of new materials with high thermoelectric performance. The success in its achievement is associated with the fulfilment of two other intermediate objectives. The first is of a methodological nature and consists on the combination of prediction models of crystalline structures with strategies for chemical-quantum calculation of electronic, thermodynamic and transport properties (VASP+newGIBBS). The second is of an applied nature. It seeks to obtain property-structure correlations from the computational exploration of regions of increasing pressures in the phase diagram of families of compounds with high value of the figure of merit (ZT) (AgCl, PbTe, SnSe, CoSb3) and allowing stoichiometric variations. The code XtalOpt is a computational tool that makes use of evolutionary algorithms for the prediction of crystal structures based solely on the composition of a material system. The number of atoms in the unit cell that handles. XtalOpt can reach a hundred. It has been created entirely of Prof. Eva Zurek. Its set up to couple it with the code GIBBS2 supposes a novel computational strategy in the search for stable structures in specific regions of the phase diagram, created in the group TCCMAT at the University of Oviedo. Hocine C has completed his PhD at the age of 45 years from Oviedo University, Spain. He is professor of Université des frere Mentouri, Constantine/Algeria. He has over 5 publications that have been cited over 20 times, and his publication H-index is 7.8.

Recent publications

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