Aims and Scope:

The usage of physical information in quantum mechanics is important for the ramification of the theoretical models dealing with the micro-domain of the nature. Some key components of conceptual constructs of chemistry and physics are atomic radius, electronegativity, the global hardness and the global electrophilicity index. These ingredients are fundamentally atomic descriptors and are carrying physical or quantum information of physical or quantum systems—the atoms into the molecules. The descriptors of conceptual constructs of chemistry and physics find application in the real world of chemistry and physics. Their importance can be assessed by simply noting that without the concept and operational significance of radius, hardness and electronegativity the chemistry and many aspects of condensed matter physics become chaotic and the long established unique order in chemico-physical world would be disturbed. But when their fundamental status in science is enquired it is transparent that, in spite of their manifold applications in the chemico-physical world, none of the descriptors—the radius, the electronegativity, the hardness and electrophilicity index has ever been measured experimentally as because none of them is physical observable. Thus they may be considered as mythical saga or Kant’s Neumann ie they exist in mind not in the real world. Moreover, since the descriptors are not observables, according to the rules of quantum mechanics, no operator can be suggested for their quantum mechanical evaluation. Hence these important and indispensable descriptors are basically qualitative per se. However, the conceptual density functional theory has developed theoretical algorithms to evaluate such descriptors and when these numerical values are applied to study chemico physical phenomena we get encouraging results.

Dates:

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