



Contribution ID: 30

Type: **not specified**

On measuring localization and delocalization patterns in molecules

Tuesday, 17 March 2026 15:30 (12 minutes)

After a brief introduction about the quantum 20th century, and about the year of 2025 as the international year of quantum theory and quantum technology, according to the United Nations resolution, we begin to discuss the impact of the former and its two key narratives – the observer and the measurement - on quantum chemistry and its core concepts: the bond, localization and delocalization. We demonstrate that the latter two took the origin in the old quantum theory that started in 1900, in M. Planck's hands. The above narratives were marked by J. Bell in his work "Against 'measurement'", where he mentioned P.A.M. Dirac as the most distinguished of 'why bother?'ers since P. Dirac in his paper "The Evolution of the Physicist's Picture of Nature" considered the difficulties of quantum mechanics and divided them into two classes. Into the first one, he particularly attributed the problems of 'observer' and 'measurement' and suggested that these problems should be left for later. It is precisely the latter that is the goal of this work that splits into two goals. The first is to construct a logically consistent chain of reasoning to link to the above narratives. The second is to propose a new model of quantum measurement based on the concept that the state of a quantum system necessarily changes under measurement, that put forward in the works of Fock, von Neumann and De Broglie, and many others and that aims to measure quantum chemical localization and delocalization patterns. The latter particularly describes the formation of the hydrogen bond. The measuring protocol is performed via the measurement machine that particularly employs the architecture of neural networks.

Presenter: Prof. KRYACHKO, Eugene (Boglyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine)