

On processes of structure formation - a fundamental new approach -

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The formation of crystalline structures is far from being well understood. A cloud of atoms condenses to a liquid and at lower temperature forms a crystal. Quantum chemistry, statistical physics, as well as thermodynamics all play an indispensable role but, each of them is unable to solve the problem alone. Here we describe structure formation along the formal language of thermodynamics, but, as far as we know, for the first time by an extended version (*General Dynamics*) applied to internal subsystems. The extension originates from Gibbs complete fundamental form, and hence includes momentum as well as angular momentum, both included in quantum chemistry and statistical physics too, but not in classical thermodynamics. General Dynamics, hence, has the potential to bridge the gap between quantum chemistry and thermodynamics, will be able to describe the path matter goes from individual atoms to a crystal.

Liquid and amorphous systems are intermediate phases, are precursors of any crystalline state. They show well defined short-range order treatable by quantum chemistry. But, their medium-range order shows features which are different, can not, or only partly be understood by local quantum chemistry. The fundamental processes causing these medium-range features may help us to understand the formation of long-range structural order.

Over the years we could show that liquid and amorphous systems, irrespective whether they are elementary, binary, or ternary, metallicly, covalently as well as ionically bonded, that major structural features are formed under the influence of resonances between global subsystems as there are all the electrons as one, and the forming static structure as the other one. The resonances mentioned are in particular dominating the medium range. Accordingly, for a complete description of structure formation, global effects have to be taken into account in addition to local quantum chemistry, both have to go hand-in-hand. The global subsystems adjust mutually their internal parameters and cause spherical periodic order (SPO) in the mean around any atom.

We discuss resonances based on momentum exchange as the driving effect, causing anti-bonding (non-equilibrium) as well as bonding (equilibrium) states between the global subsystems with a gap or pseudogap at E_F in-between, with all the consequences on phase stability and electronic transport. We discuss the importance of the creation of entropy whenever the system finally transfers to the bonding state, forms (occasionally) a new material or a new crystal.