

## **Comprehensive Application of LFES-Principles in New Computer Modeling Technologies**

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Analysis of various methods of computation of thermodynamic kinetic characteristics of hydrocarbons and organic reactions allowed to recognize that all them are governed by a common rule of linear-free energy ship (LFES) over a wide range of temperatures and pressure. As for hydrocarbon compounds (C-H-O-N-S) it was determined that this rule may be observed in hydrocarbons with a wide range of C<sub>1</sub>-C<sub>100</sub> quantities in the form of one-, two-,and multi-characteristic linearity.

Comprehensive application of LFES- principle in combination with comparative and other computational methods used to calculate thermophysical, physics-chemical, molecular and thermochemical properties allows to obtain all data necessary for computer modeling of the formation and transformation processes for oil, gas, coals and shales in a multi-phase and heterogeneous system of hydrocarbons-organic remains-enclosing (country) rocks-formation waters.