

# Quantum Chemistry at the high pressures: the eXtreme Pressure Polarizable Continuum Model (XP-PCM).

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The eXtreme-Pressure-Polarizable Continuum Model is aimed to the study of the effects of high pressure on molecular properties and processes [1]. The XP-PCM method has been systematically developed for several quantum chemical levels, including coupled-cluster methods, along with the corresponding analytical derivatives of the energy for the calculation of the equilibrium geometry and molecular response functions under high pressure. The method has been applied to several molecular properties under pressure, such as the IR/Raman vibrational frequencies [2], electronic excitations [3]. The XP-PCM method also allows for the study of the effect of the pressure on the potential energy surface of chemical reactions [4, 5], including the quantum chemical calculation of the activation volumes. More recently, it has been applied to the study of the effect of the pressure on the electron configuration and electronegativity of 93 elements of the periodic table. [6].

In this short communication, we will spot on essential aspects of the XP-PCM theory and some of its applications.

References:

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