Contribution ID: **95** Type: **Poster**

Electronic structures and optical properties of different phases of polyvinylidene fluoride (PVDF) crystals

Friday, November 8, 2024 4:42 PM (3 minutes)

Polyvinylidene fluoride (PVDF) is an organic polymer that exhibits significant potential and commercial appeal for modern applications in nanotechnology, microelectronics, and biomedicine. A real PVDF polymer is almost always a mixture of several polymorphic phases that are difficult to separate. Determining the phase composition of PVDF mixtures is a critical technological task. This report presents results of the ab-initio calculations of the electronic band structures of the three most common phases of PVDF crystals: α-, β-, and γ-PVDF. The results include the one-electron band structures (band dispersion curves), partial densities of electronic states, spatial distributions of electron density, spectra of dielectric constants, complex refractive indices, absorption and reflection spectra, infrared absorption, Raman scattering, and X-ray diffraction patterns for the α-, β-, and γ-phases of PVDF. The analysis of the electronic structure calculations allowed to make several conclusions regarding the formation of electronic and optical properties of the α-, β-, and γ-phases of PVDF, as well as predictions about the potential for experimental monitoring of the phase composition of this compound. It was established that detecting the simultaneous presence of β- and α-(or γ-) phases in PVDF crystal samples can be effectively achieved using reflection spectroscopy in the vacuum ultraviolet range, infrared absorption, Raman scattering, and X-ray phase analysis. However, distinguishing the presence of the α-phase against the background of the γ-phase using these methods would be practically impossible.

Type of presence

Presence at Taras Shevchenko National University

Primary author: BARANCHICOV, Zahar (student)

Co-authors: Mr MAKARENKO, Oleksii; Prof. NEDILKO, Serhii (Taras Shevchenko National University of Kyiv); HIZHNYI, Yuriy (Taras Shevchenko National University of Kyiv)

Presenter: BARANCHICOV, Zahar (student)

Session Classification: Poster Session