&RPSXWDWLRQDO VWXGLHV RI IHUURHOHFWULF FRPSRVLWHV (PVDF) and graphene/graphene oxide

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Computational molecular investigations and experimental studies of the ferroelectric properties of new composite nanomaterials based on polymer ferroelectrics and graphene/graphene oxide are presented. Main results of the computational molecular modeling of various nanostructures and the piezoelectric properties of the composites from polyvinylidene uoride (PVDF)/poly(vinylidene uoride-tri uoroethylene) (P(VDF-TrFE)) lms and graphene/graphene oxide (G/GO) were reviewed and analyzed in comparison with the experimental data at the nanoscale, particularly with atomic force and piezo-response force microscopy (AFM/PFM) data. e performed computational molecular modeling of the graphene/ graphene oxide (G/GO) and PVDF ferroelectric polymer composite nanostructures were studied by the di erent methods using HyperChem tool: molecular mechanics (MM) methods (BIO CHARM), quantum mechanical (QM) calculations based on density functional theory and semi-empirical PM3 method. Experimentally the switching behavior, piezoelectric response, dielectric permittivity and mechanical properties of the lms were investigated and found to depend on the presence of G/ GO concentration variation. Experimental results qualitatively correlate with those obtained in the calculations. Particularly, computed data of the piezoelectric coe cients d33 for developed PVDF-G/GO models are in line with observed experimental behavior with concentration changes of GO components. Further development with several multilayered GO nanostructures and inserted PVDF chain and layers, having new curved structures a er optimization are considered and discussed. e properties of these investigated nanostructures with the GO content dependence for these composites are analyzed. e results obtained in the reviewed and analyzed present study provide important insights into our understanding of the mechanisms of piezoelectricity in such new nanocomposites give us new prospective for further creation, development and applications of novel ferroelectric polymer–graphene/graphene oxide nanocomposites as multifunctional nanomaterials.

Recent Publications

1. Bystrov V S, Bdikin I K, Silibin V, Karpinsky D, Kopyl S, Goncalves G, Sapronova A V, Kuznetsova T and Bystrova V V (2017) Graphene/graphene oxide and polyvinylidene uoride polymer ferroelectric composites for multifunctional applications. Ferroelectrics 509(1):124-142.
2. Paramonova E V, Filippov S V, Gevorkyan V E, Avakyan L A, Meng X J, Tian B B, Wang J L and Bystrov V S (2017) Polarization switching in ultrathin polyvinylidene uoride homopolymer ferroelectric lms. Ferroelectrics 509(1):143–157.
3. Bystrov V S, Paramonova E V, Bdikin I K, et al. (2013) Molecular modelling of the piezoelectric e ect in the ferroelectric polymer poly(vinylidene uoride) (PVDF). J. Mol. Mod. 19(9):3591-3602.
4. Bystrov V S (2014) Molecular modeling and molecular dynamic simulation of the polarization switching phenomena in the ferroelectric polymers PVDF at the nanoscale. Physica B: Condensed Matter 432:21-25.

Biography

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