

**Broadband Negative Epsilon at Visible Spectrum with Ag@SiO₂ Core-Shell Nanoparticles/Polymer Composites Using Machine Learning Approach****Zahra Lalegani, Mohammad Hossein Golbabaie, Seyyed Ali Seyyed Ebrahimi***Advanced Magnetic Materials Research Center, School of Metallurgy and Materials, College of Engineering, University of Tehran, Tehran, 11155 4563, Iran***Abstract**

In this study, the prediction of the composition and geometry of a polymer composite film containing Ag@SiO₂ core-shell nanoparticles (NPs) was investigated in order to achieve the property unavailable in nature of negative epsilon for optical applications. A machine learning approach was used for prediction, and this work was carried out in two sections: prediction of Stöber synthesis conditions of Ag@SiO₂ NPs to achieve the desired geometry of core-shell NPs; and prediction of optimal geometrical conditions for a polymer matrix composite film containing Ag@SiO₂ core-shell NPs, to achieve negative epsilon in the visible spectrum. In this regard, a dataset collected from various experimental studies containing some 450 samples was used, which covered synthesizing and composite fabrication parameters. An optimization procedure was implemented to find the best neural networks architecture to induce two models with high predictive performance. The built neural network could correctly predict the SiO₂ shell thickness with 0.997 accuracy, whereas 87% of the data were predicted with an absolute error lower than 1 nm. Also, the second resulting neural network could predict the epsilon-effective of composite film with 0.997 accuracy, whereas 98% of the predicted data have an absolute error lower than 0.5. The most important achievement of this study was the model's ability to predict the target values, which were not included in the experimental dataset used for training, which showed an excellent generalization ability. This study could be a general solution and the basis of future studies in predicting negative epsilon composites containing different core-shell NPs and will open the way for designing new materials.

Biography

Dr. Lalegani, holder of a Ph.D. in materials engineering from the University of Tehran, is experienced in materials processing and characterization. In her prior research activities, she has studied the synthesis of nanomaterials using DoE. Now, she is working on optimization of materials properties using machine learning.