

Discovery of novel oxynitride phosphors for use in LEDs

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We employed heuristics optimization involving the parameterization of material novelty. Heuristics optimization strategies such as a non-dominated sorting genetic algorithm (NSGA) and particle swarm optimization (PSO) were coupled with high-throughput experimentation (HTE), in such a manner that the experimental evaluation of fitness functions for NSGA and PSO was accomplished by HTE. We used a non-dominated sorting genetic algorithm (NSGA) for a preliminary screening of a multi-dimensional search space, and particle swarm optimization (PSO) for the ensuing fine-tuning in a reduced composition space to narrow the possibility of discovery. The proposed strategy also involves the parameterization of material novelty to systematically avoid a futile convergence on well-known, already-established materials. For this sake, we also created a parameter designating the novelty of phosphors, the so-called structural rank, and used it as an objective (fitness) function in NSGA. As a result, we discovered several novel, single-phase, phosphors, which have strong potential for practical use in white light-emitting diodes and thereby is ready for commercialization.