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Sommario/riassunto	The title of the current Special Issue, "Feature Papers in Materials Simulation and Design", has identified the aims of this collection since its opening: the gathering of research works and comprehensive review papers that advance the understanding and prediction of material behavior at different scales, from atomistic to macroscopic, through innovative modeling and simulation.In this context, interdisciplinary researches that tackled challenging and complex material problems where the governing phenomena might span different scales of material behavior, with an emphasis on the development of quantitative approaches to explain and predict experimental observations, have been collected. Similarly, particular attention has been given to homogenization techniques for the evaluation of the mechanical properties of new materials and multi-phase composites. Innovative numerical approaches for the mechanical analysis, highlighting their accuracy, reliability, and stability features, have been also welcomed. Significant space has been also given to advanced and sustainable technologies. From the aforementioned topics, it is evident that this Special Issue represents the ideal forum for disseminating excellent research findings, as well as sharing innovative ideas in this significant field.Throughout the several months of activity, this Special Issue has been able to attract much interesting research. Its success is proven by the sixteen papers collected and published.