

## Special Issue on Materials Design and Simulation

### Call for Papers

To understand the chemical and physical phenomena used in materials for energy conversion and chemical reaction, it is necessary to apply computer simulation. The ability to design new materials which with high-performance and high-function from quantum mechanical principles with computers is currently one of the fastest growing and most exciting areas of theoretical research in the materials science. Examples include modeling of chemical reaction, computation of aerospace instruments, design of new alloys and multilayers, and processing of semiconductors.

In this special issue, we intend to invite front-line researchers and authors to submit original researches and review articles on exploring **materials design and simulation**. Potential topics include, but are not limited to:

- Design and manufacturing systems
- Process modeling, analysis and simulation
- System modeling
- Computer aided design of materials
- Simulation technology
- Intelligent materials design
- Modeling of novel material systems

Authors should read over the journal's [For Authors](#) carefully before submission. Prospective authors should submit an electronic copy of their complete manuscript through the journal at [Paper Submission System](#).

Please kindly specify the “**Special Issue**” under your manuscript title. The research field “**Special Issue – Materials Design and Simulation**” should be selected during your submission.

Special Issue timetable:

Submission Deadline	September 26th, 2017
Publication Date	November 2017

#### Guest Editor:

For further questions or inquiries  
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