

PRESS RELEASE
Frankfurt am Main, Germany (July 6th, 2016)

Why is alloy theory still a matter of principles?

Plenary Lecture by **Patrice E. A. Turchi** (*Lawrence Livermore National Laboratory*)

Wednesday, September 28th, 2016, 2:00 p.m. - 2:30 p.m., Audimax, TU Darmstadt



Ab initio methodologies provide, in spite of their own limitations that will be briefly commented on, fundamental insight on various materials characteristics. This will be illustrated in the case of chemical-order trends and thermodynamic properties with ab initio-based predictions.

In addition, ab initio output plays an important role in supplementing in two ways CALPHAD that is the most versatile and preferred method for assessing the thermodynamics of complex multi-component alloys: either by direct input of ab initio energetics in thermodynamic databases, or, more challenging, by assessing ab initio-based thermodynamics à la CALPHAD. These two applications will be discussed in the context of phase diagram determination for selected transition metal and actinide-based alloys. Finally a few comments on future prospects in the alloy theory field, of critical importance for advancing materials design, will conclude this presentation.

Work performed under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA27344.

Topics: ab initio calculations, ground-state properties, thermodynamics, multi-component alloy

For more information on our plenary lectures please visit our [website](#). If you wish to register as a media representative and get free access to MSE 2016 please contact us directly at presse@dgm.de.

Further plenary lectures include:



Peter Greil (University of Erlangen-Nuernberg, Department of Materials Science (Glass and Ceramics), Erlangen, Germany):

Biomorphous Ceramics

Tuesday, September 27th, 2016, 10:00 a.m. - 10:30 a.m.



Jörg F. Löffler (Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, Switzerland):

Metallic biomaterials for absorbable implant applications

Tuesday, September 27th, 2016, 1:45 p.m. - 2:15 p.m.



Yuri Estrin (Department of Materials Science and Engineering, Monash University, Clayton, Australia):

Ultrafine grained metallic materials for permanent and bioresorbable medical implants

Wednesday, September 28th, 2016, 8:30 a.m. - 9:00 a.m.



Laurent Pambaguian (Engineer in the Materials Technology Section of the European Space Agency, Netherlands):

Additive Manufacturing for space industry

Wednesday, September 28th, 2016, 6:15 p.m. - 6:45 p.m.



Christoph Bartneck (HIT Lab NZ, University of Canterbury, Christchurch, New Zealand):

Material Challenges in Human Robot Interaction

Thursday, September 29th, 2016, 8:30 a.m. - 9:00 a.m.



Cesar A. Barbero (Department of Chemistry, Universidad Nacional de Rio Cuarto, Rio Cuarto, Argentina):

Smart Polymeric Nanocomposites and Polymer Alloys. Synthesis and Applications

Thursday, September 29th, 2016, 2:00 p.m. - 2:30 p.m.

About MSE 2016 - <https://www.mse-congress.de/home/>

Once again the time has arrived: from September 27th to 29th, 2016 Europe's Material Science and Engineering scientists (MatWerk) will meet at the Materials Science and Engineering Congress (MSE) at the Darmstadt University of Technology, Germany. A special highlight is this year's guest country, one of the most important research and economic regions in the world, the USA.

With more than 1,400 participants, the MSE is one of the largest English speaking congresses with exhibition in the field of Material Science and Engineering across Europe. In symposia and plenary lectures numerous scientific, social and economic relevant questions of Material Science and Engineering are discussed every two years.

For 2016 the biggest U.S. societies: the Materials Research Society (MRS) and the Minerals, Metals and Materials Society (TMS) have been involved in the concept and design of the congress.

Hosted by the German Materials Society (DGM) in Darmstadt, Germany the MSE is the central platform for material science and engineering experts to present their research field to a large international community and to network across borders since 2008. In addition to different side events, the DGM Tag with its Nachwuchsforum is an integral part of the MSE.

The MSE's host, the DGM, is the largest technical-scientific society for Materials Science and Engineering in Europe. For almost 100 years it has combined the expertise of the specialist field from science and the industry: by representing the interests of its members from science and the industry - and acting as a guarantor for the systematic development of the field.

Comprehensive information on the [highlights of this year's MSE](#) and a [program overview](#) can be found online.

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