



### **MmeEgp02-001**

#### **Machine learning approaches to optimize materials research**

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Keynote: The development of new materials and production processes and the customization of existing ones are increasingly driven by AI, in particular Bayesian optimization and surrogate modeling. In many cases, materials science has relied on compute-intensive simulations to evaluate the properties of proposed designs or the effect a change might have. Such simulations do not scale to the vast design spaces that materials scientists explore. Machine learning provides an alternative: properties are approximated through the predictions of surrogate models rather than computed by simulations, orders of magnitude faster. Both AI and materials science are working on conceptually similar problems – how to efficiently identify the best design choices, be that for a machine learning pipeline or a new material. Yet, there is little collaboration between the communities. The purpose of this workshop is to bring the communities closer together, facilitate cross-disciplinary collaborations, identify common problems, and develop plans for tackling them.