

# Machine Learning for Materials Hard and Soft

## ESI-DCAFMTACO\_VDSP Summer School 2022

### Schedule – Week 1

	Mon, 11 Jul	Tue, 12 Jul	Wed, 13 Jul	Thu, 14 Jul		Fri, 15 Jul
09.00	“Mathematical Introduction I” <b>Philipp Grohs</b> University of Vienna	“Mathematical Introduction II” <b>Philipp Grohs</b> University of Vienna	“Image Analysis” <b>Thomas Pock</b> TU Graz	“ML for electronic structure” <b>James Spencer &amp; David Pfau</b> Deep Mind	09.00	<b>Bingqing Cheng</b> Institute of Science and Technology Austria (ISTA)
					09:45	<b>Andrew Ferguson</b> University of Chicago
10.30	<i>Coffee Break</i>	<i>Coffee Break</i>	<i>Coffee Break</i>	<i>Coffee Break</i>	10.30	<i>Coffee Break</i>
11.00	“Mathematical Introduction I” <b>Philipp Grohs</b> University of Vienna	“Mathematical Introduction II” <b>Philipp Grohs</b> University of Vienna	“Image Analysis” <b>Thomas Pock</b> TU Graz	“ML for electronic structure” <b>James Spencer &amp; David Pfau</b> Deep Mind	11.00	<b>Marjolein Dijkstra</b> University of Utrecht
					11.45	“AI Case Studies” <b>Marine Pigneur</b> (MLR GmbH) <b>Christopher Lepenik</b> (Image Biopsy Lab) <b>Christian Leitold</b> (Verbund) <b>Bhuiyan S.M. Ebna-Hai</b> (Fehrmann)
12.30	<i>Lunch Break</i>	<i>Lunch Break</i>	<i>Lunch Break</i>	<i>Lunch Break</i>	12.45	<i>AI Lunch</i>
14.00 – 17.00	Tutorial <b>Philipp Grohs</b> University of Vienna	Tutorial <b>Philipp Grohs</b> University of Vienna	Tutorial <b>Thomas Pock</b> TU Graz	Tutorial <b>James Spencer &amp; David Pfau</b> Deep Mind	14.30	<b>Milica Todorovic</b> University of Turku
					15.15	<b>Reinhard Maurer</b> University of Warwick
17.00	<i>Welcome reception</i>				16.00	<b>Roberto Covino</b> Frankfurt Institute for Advanced Studies (FIAS)

**Registration:** Monday, 11 July 2022, at 08.30 in front of ESI Boltzmann lecture hall, top floor, ESI, Boltzmanngasse 9a, 1090 Vienna

**Lectures:** ESI Boltzmann lecture hall | **Tutorials:** ESI Boltzmann & ESI Schrödinger lecture halls | **Coffee Break:** ESI common room | **Lunch Break:** self-organized

# Machine Learning for Materials Hard and Soft

## ESI-DCAFM-TACO\_VDSP Summer School 2022

### Schedule – Week 2

	Mon, 18 Jul	Tue, 19 Jul	Wed, 20 Jul	Thu, 21 Jul	Fri, 22 Jul
09.00	“ML potentials” <b>Philipp Marquetand</b> University of Vienna	“ML potentials” <b>Philipp Marquetand</b> University of Vienna	“Statistical Sampling” <b>Peter Wirnsberger</b> Deep Mind	“Free energies and enhanced sampling” <b>Luigi Bonati</b> IIT Genova	“Materials properties prediction” <b>Taylor D. Sparks</b> University of Utah
10.30	<i>Coffee Break</i>	<i>Coffee Break</i>	<i>Coffee Break</i>	<i>Coffee Break</i>	<i>Coffee Break</i>
11.00	“ML potentials” <b>Philipp Marquetand</b> University of Vienna	“ML potentials” <b>Philipp Marquetand</b> University of Vienna	“Statistical Sampling” <b>Peter Wirnsberger</b> Deep Mind	“Free energies and enhanced sampling” <b>Luigi Bonati</b> IIT Genova	“Materials properties prediction” <b>Taylor D. Sparks</b> University of Utah
12.30	<i>Lunch Break</i>	<i>Lunch Break</i>	<i>Lunch Break</i>	<i>Lunch Break</i>	<i>Closing Remarks</i>
14.00 – 17.00	Tutorial <b>Philipp Marquetand</b> University of Vienna	Tutorial <b>Philipp Marquetand</b> University of Vienna	Tutorial <b>Peter Wirnsberger</b> Deep Mind	Tutorial <b>Luigi Bonati</b> IIT Genova	
18.00		<i>Social Dinner</i>			

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**Lectures:** ESI Boltzmann lecture hall | **Tutorials:** ESI Boltzmann & ESI Schrödinger lecture halls | **Coffee Break:** ESI common room | **Lunch Break:** self-organized