2022 ATOMIC LAYER PROCESSING MODELLING WORKSHOP

March 15

Time	Title	Speaker
13:00	*Opening talk*	Henrik Pedersen, Linköping Univeristy
13:10	*A mechanistic study of the HF pulse in the thermal atomic layer etch of crystalline and amorphous HfO2*	Rita Mullins, Tyndall National Insitute
13:25	*Atomic-scale modelling applied to the understanding of indium nitride growth by atomic layer deposition methods*	Giane B. Damas, Linköping University
13:40	*First principles modelling of growth of Al2O3-based hybrid films*	Arbresha Muriqi, Tyndall National Insititute
13:55	*Break*	
14:10	*Computational investigation of precursor blocking by aniline inhibitor molecules during area-selective atomic layer deposition*	Ilker Tezsevin, Eindhoven University of Technology
14:25	*On the accuracy of density functional theory in prediction of Cu ALD and ALE reaction energies*	Xiao Hu, Fraunhofer ENAS
14:40	*Modelling the atomic layer deposition of cobalt and ruthenium on NHx-terminated Metal Surfaces*	Ji Liu, Tyndall National Institute
14:55	*Break*	
15:20	*First-principles framework for surface-assisted dissociative adsoption dynamics*	Mateusz Wlazlo, CBRTP
15:35	*Film growth modelling through coupling of particle Monte Carlo and Level set methods*	Joshua Gehre, Fraunhofer ENAS
15:50	*Break*	
16:15	**Tutorial:** *Reaction network analysis of ALD processes: Is this a true ALD cycles? What rates can be measured?*	Raymond Adomaitis, University of Maryland

March 16

Time	Title	Speaker
08:30	*Influence of flow regime on the conformality of atomic layer depositoin in lateral channels: simulations with a diffusion-reaction model*	Jorge A. Velasco, Aalto University
08:45	*Computational fluid dynamics modeling of spatial atomic layer deposition on microgroove substrates*	Zoushuang Li, Huazhong Univeristy
09:00	*Break*	
09:15	*Numerical simulations of atomic layer deposition process*	Gizem Ersavas Isitman, Aalto University
09:30	*A call to establish best practice guidelines for reactor-scale simulations*	Anton Persson, Linköping University
09:50	*Break*	
10:20	*Investigating the limitations of plasma-enhanced atomic layer deposition of silver films using lateral high aspect ratio microstructures*	Renaud Leturcq, LIST
10:40	*In-situ metrology for atomic layer processes*	Martin Knaut, TU Dresden/ALS Metrology
11:00	*Atomic-scale simulation frameworks for ASD*	Umberto Martinez, Synopsys
11:20	*Break*	
11:35	*Picosun's view on the current state of the art and further development needs in modelling ALD processes*	Tom Blomberg, Picosun Oy
11:55	*Validation issues for atomic-scale simulations of atomic layer processing*	Simon Elliott, Schrödinger
12:15	*Closing*	Anton Persson, Linköping University

Main industrial partner:

Main academic partner: