

# Monday, January 25, 2021

**10:00 - 10:10**

## Welcome Addresses

Bernhard L.A. Pichler and Wolfgang Dienemann

Zoom

**10:10 - 11:10**

## Nucleation and growth of C-S-H: Nanoengineering of cementitious materials

Chairperson: Karen Scrivener

Zoom

10:10	<b>J. Li, K. Xu, P. Monteiro:</b> Fibrillar C-S-H seed from hydrated C3S accelerates cement hydration	21
10:20	<b>M. N. Harris, K. Scrivener, P. Bowen:</b> A recipe for the reliable and reproducible precipitation of pure phase, high Ca:Si ratio (>1.5) synthetic calcium silicate hydrates (C-S-H)	23
10:30	<b>J. Plank, M. Theobald, V. Kanchanason:</b> Insights into the very early nucleation and growth of C-S-H in the presence and absence of superplasticizers	25
10:40	<b>A. Morales Melgares, P. Moutzouri, P. Bowen, E. Lyndon, K. Scrivener:</b> Zn incorporation in synthetic C-S-H and its effect on cement hydration through DNP enhanced MAS NMR	27
10:50	<b>F. Zunino, K. Scrivener:</b> The influence of gypsum addition on the early age hydration of C3S systems	29
11:00	<b>Plenary Discussion</b>	

**11:10 - 11:30**

## Interactive Discussion

Gather.Town

## 11:30 - 12:30

### Nucleation and growth of C-S-H: Nanoengineering of cementitious materials

Chairperson: Paul Bowen

Zoom

11:30	<b>F. Kleiner, C. Rößler:</b> Utilizing modern FIB/SEM technology and EDX for three-dimensional imaging of hydrated alite and its pore space	31
11:40	<b>L. Nguyen-Tuan, M. Etzold, C. Rößler, H.-M. Ludwig:</b> Simulation of the C-S-H nucleation and growth using fiber elements	33
11:50	<b>X. Mendez Aretxabaleta, J. López-Zorrilla, I. Etxeberria, H. Manzano:</b> The formation of C-S-H from portlandite nanoclusters: clues from atomistic simulations	35
12:00	<b>M. Valavi, S. Galmarini, A. Kunhi Mohamed, P. Bowen:</b> Development and application of new force field suite for atomistic simulations of cementitious materials	37
12:10	<b>Z. Casar, A. Kunhi Mohamed, K. Scrivener, P. Bowen:</b> Atomistic modeling of calcium silicate hydrate	39
12:20	Plenary Discussion	

## 12:30 - 12:50

### Interactive Discussion

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12:50

## Lunch Break

## 14:00 - 15:00

Zoom

**Invited talks:**  
**Thermodynamics of Calcium-Aluminate-Silicate-Hydrates**  
 Chairperson: Barbara Lothenbach

14:00	<b>A. Kunhi Mohamed:</b> Atomic-level structural features of C-(A)-S-H	41
14:30	<b>C. S. Walker, S. Anraku, H. Sasamoto, M. Mihara:</b> C(-A)-S-H gel solubility model development and its application to high content fly ash silica fume cement	43

15:00

## Break

## 15:10 - 16:20

Zoom

**Thermodynamics of Calcium-Aluminate-Silicate-Hydrates**  
 Chairperson: Jørgen Skibsted

15:10	<b>S. Barzgar, B. Lothenbach, M. Tarik, C. Ludwig:</b> The effect of pH, Ca/Si ratio and equilibration time on Al uptake in calcium silicate hydrates (C-S-H)	45
15:20	<b>S.-Y. Yang, Y. Yan, B. Lothenbach, J. Skibsted:</b> Structural characterization of synthesized calcium alumina-silicate hydrate (C-A-S-H) phases by the solid-state NMR	47
15:30	<b>N. Chitvoranund, B. Lothenbach, K. Scrivener:</b> C-(A)-S-H formation of high Al systems in real microstructure	49
15:40	<b>Y. Yan, B. Lothenbach, K. Scrivener:</b> Effect of alkali hydroxide on calcium silicate hydrate	51
15:50	<b>G. D. Miron, D. A. Kulik, B. Lothenbach:</b> Incremental parameterisation of CASH+ sublattice solid solution model against recent data for Na, K, and Al uptake in C-S-H	53
16:00	<b>P. Blanc, A. Lach, A. Lassin, S. Guignot:</b> Modeling hydration of mine tailings: production of hydraulic binders from alkali-activated materials	55
16:10	<b>Plenary Discussion</b>	

## 16:20 - 16:40

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### Interactive Discussion

# Tuesday, January 26, 2021

## 10:00 - 11:00

Zoom

**Invited talks:**  
**Nanoscale phenomena during the first and subsequent sorption cycles**  
 Chairperson: Mohsen Ben Haha

10:00	<b>I. Maruyama, R. Kurihara, T. Fujimaki:</b> Shrinkage of C3S paste associated with a dynamic microstructure change under the first drying	57
10:30	<b>J. Adolphs:</b> Water vapor sorption and in situ determination of swelling and shrinkage of hardened cement paste	59

11:00

## Break

## 11:10 - 12:10

Zoom

**Nanoscale phenomena during the first and subsequent sorption cycles**  
 Chairperson: Jürgen Adolphs

11:10	<b>A. Nagmutdinova, V. Bortolotti, L. Brizi, P. Fantazzini:</b> Characterization of first sorption cycle by 1h NMR: quantitative analysis of nano-porous structure and solids in cement materials	61
11:20	<b>M. Rastogi, A. Müller, M. Ben Haha, K. Scrivener:</b> Insights on desorption of calcium silicate hydrate	63
11:30	<b>L. Huang, L. Tang, I. Löfgren, O. Nilla:</b> Water distribution in green cementitious materials under different relative humidity	65
11:40	<b>T. Honorio, Z. Shi:</b> Sorption and specific ion effects in crystalline ASR products studied using molecular simulations	67
11:50	<b>N. Krattiger, B. Lothenbach, S. V. Churakov:</b> Sorption and electrochemical properties of ASR products and C-S-H: a comparative modelling study	69
12:00	<b>Plenary Discussion</b>	

## 12:10 - 12:30

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### Interactive Discussion

12:30

## Lunch Break

## 13:30 - 14:30

Zoom

**Invited talks:**  
**Transport of water and small ion through agglomerates of hydrates**  
 Chairperson: Peter J. McDonald

13:30	<b>C. Hall:</b> Contact time: capillary transport with material alteration	71
14:00	<b>N. M. Alderete, R. Patel, Y. Villagrán Zaccardi, N. De Belie:</b> Understanding deformations in cementitious materials during capillary imbibition	73

14:30

## Break

## 14:40 - 15:50

Zoom

**Transport of water and small ion through agglomerates of hydrates**  
 Chairperson: John Provis

14:40	<b>O. Istok, M. Janota, A. M. Gajewicz-Jaromin, P. J. McDonald, D. A. Faux, H. S. Wong, M. H. Yio:</b> MRI studies of water sorption and dynamic porosity in cement pastes at micro and macro scale: 1 - results	75
14:50	<b>M. Janota, O. Istok, A. M. Gajewicz-Jaromin, P. J. McDonald, D. A. Faux, H. S. Wong, M. H. Yio:</b> MRI studies of water sorption and dynamic porosity in cement pastes at micro and macro scale: 2 - discussion	77
15:00	<b>M. N. Borg, D. A. Faux, P. J. McDonald:</b> Lattice Boltzmann modelling of water transport in hydrates agglomerates	79
15:10	<b>Z. Zhakiyeva, A. Fernandez-Martinez, A. Van Driessche, G. Cuello, F. Claret, I. Bourg, H. Fischer:</b> The structure of water in calcium-silicate-hydrates studied by neutron diffraction with isotopic substitution	81
15:20	<b>A. Abdu Rahaman, D. A. Faux, P. J. McDonald, O. Istok, D. Brougham, E. McKiernan:</b> Nuclear spin relaxation in aqueous paramagnetic ion solutions	83
15:30	<b>R. Kogon, P. Fantazzini, L. Brizi, V. Bortolotti, D. A. Faux, P. J. McDonald:</b> 3 Tau Model: Implementation of new features to the 3TM script and examples of application to cement paste dispersion profiles	85
15:40	<b>Plenary Discussion</b>	

## 15:50 - 16:10

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**Interactive Discussion**

# Wednesday, January 27, 2021

## 10:00 - 11:00

Zoom

**Invited talks:**  
**Transport of water and small ion through agglomerates of hydrates**  
 Chairperson: Villiam Bortolotti

10:00	<b>M. Wyrzykowski, P. J. McDonald, A. M. Gajewicz-Jaromin, D. Dunstan, K. Scrivener, P. Lura:</b> Redistribution of water in hardened cement paste under thermal and mechanical loading	87
10:30	<b>L. Pel:</b> NaCl ion transport and interaction in cementitious materials as observed by NMR	89

11:00

## Break

## 11:10 - 12:00

Zoom

**Transport of water and small ion through agglomerates of hydrates**  
 Chairperson: Bruno Huet

11:10	<b>F. Georget, C. Bénier, W. Wilson, K. Scrivener:</b> Direct observation of chloride sorption on C-S-H	91
11:20	<b>A. A. Pirvan, M. Ben Haha, K. Scrivener:</b> Transport of chloride in C-S-H microstructure with controlled Ca/Si ratio	93
11:30	<b>K. Ferjaoui, F. Georget, K. Scrivener:</b> Nanoscale modelling of ionic transport in the porous C-S-H network	95
11:40	<b>A. Machner, K. De Weerd:</b> Changes in the C-S-H composition during chloride exposure	97
11:50	Plenary Discussion	

## 12:00 - 12:20

Gather.Town

Interactive Discussion

12:20

## Lunch Break

## 13:30 - 15:00

Zoom

**Invited talks:**  
**Upscaling for applications: multiscale modeling and lab-to-market transition**  
 Chairperson: Christian Hellmich

13:30	<b>M. Vandamme:</b> Modeling how fluids deform porous materials: application to drying shrinkage	99
14:00	<b>J.-F. Barthélémy:</b> A numerical tool for an easy implementation of homogenization schemes: development and applications	101
14:30	<b>J.-F. Dufrêche:</b> Multi-scale modelling of charged porous oxides	103

15:00

## Break

## 15:10 - 16:10

Zoom

**Upscaling for applications: multiscale modeling and lab-to-market transition**  
 Chairperson: Matthieu Vandamme

15:10	<b>P. Dohnalik, O. Lahayne, L. Zelaya-Lainez, B. L. A. Pichler, C. Hellmich:</b> Grid nanoindentation of mature dental cement paste	105
15:20	<b>N. Jiménez Segura, H. Wang, C. Hellmich, B. L. A. Pichler:</b> Expansion of cement paste during isothermal adsorption: a multiscale poromechanical model	107
15:30	<b>E. Binder, M. Königsberger, C. Hellmich, B. L. A. Pichler:</b> Temperature-dependent creep of mature cement paste	109
15:40	<b>M. Königsberger, L. Göbel, L. Zelaya-Lainez, O. Lahayne, B. L. A. Pichler, C. Hellmich:</b> Nanoindentation-based multiscale micromechanics model for alkali-activated slag-fly ash mixes	111
15:50	<b>J. Rodriguez-Sanchez, M. Fedorciuc-Onisa, H. Kinoshita, J.L. Provis, S. MacLachlan:</b> Development and characterization of lightweight geopolymers for construction applications	113
16:00	<b>Plenary Discussion</b>	

## 16:10 - 16:30

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**Interactive Discussion**

## 16:30 - 16:40

Zoom

**Award for the Best Young Researcher Presentation & Conference Closing**  
 Peter McDonald and Barbara Lothenbach