The Warsaw Doctoral School in Natural and Biomedical Sciences and
the Institute of Physics PAS cordially invites you to a **SPOTLIGHT TALK**

Innovative Problems in Cementitious Materials:

Bringing Nanoscale Perspectives into Construction Problems

given by

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on 13th June 2024, 10:30 at the IF PAN Auditorium
Durations: 45 min + question time

The event will be available on ZOOM also, at this link

All Warsaw-4-Phd students (and others) very welcome!

Abstract of the talk:

In this talk I will present a few success case studies where calculations using atomistic techniques, typical of the nanoscale, have been employed to study problems in cementitious materials. I will begin by describing challenges associated with powder cement, the clinker, with compounds such as belite, which are currently a key focus in the design of low CO_2 cements [1,2]. Secondly, I will proceed to describe the compounds that are formed following the hydration of the clinker. These include the C-S-H gel, which constitutes the cement glue that holds the aggregates together, as well as other secondary compounds such as portlandite [3]. Furthermore, I will review the characterisation of the C-S-H gel using NMR techniques and how this technique can be used to define the nanoscale structure of the gel phases [4]. Finally, I will examine the potential role of nanoadditions that could be intentionally incorporated into cement pastes [5-7].

[1] Cuesta, A., Ayuela, A., & Aranda, M. A. (2021). Belite cements and their activation. Cement and Concrete Research, 140, 106319.

[2] Rejmak, P., Dolado, J. S., Aranda, M. A., & Ayuela, A. (2019). First-principles calculations on polymorphs of dicalcium silicate—Belite, a main component of Portland cement. The Journal of Physical Chemistry C, 123(11), 6768-6777.

[3] Manzano, H., Dolado, J. S., & Ayuela, A. (2009). Elastic properties of the main species present in Portland cement pastes. Acta materialia, 57(5), 1666-1674.

[4] Rejmak, P., Dolado, J. S., Stott, M. J., & Ayuela, A. (2012). 29Si NMR in cement: a theoretical study on calcium silicate hydrates. The Journal of Physical Chemistry C, 116(17), 9755-9761.

[5] Ayuela, A., Dolado, J. S., Campillo, I., De Miguel, Y. R., Erkizia, E., Sánchez-Portal, D., ... & Echenique, P. M. (2007). Silicate chain formation in the nanostructure of cem.ent-based materials. The Journal of chemical physics, 127(16).

[6] Manzano, H., Enyashin, A. N., Dolado, J. S., Ayuela, A., Frenzel, J., & Seifert, G. (2012). Do cement nanotubes exist?. Advanced Materials, 24(24), 3239-3245.

[7] Izadifar, M., Dolado, J. S., Thissen, P., Ukrainczyk, N., Koenders, E., & Ayuela, A. (2023). Theoretical elastic constants of tobermorite enhanced with reduced graphene oxide through hydroxyl vs epoxy functionalization: a first-principles study. The Journal of Physical Chemistry C, 127(36), 18117-18126.

Andrés Ayuela got his PhD in physics at University of Valladolid in 1995. He was postdoctoral reasercher at Dresden University in Technology in 1996 – 1997, in 1998 – 2003 he was reasercher at Helsinki University of Technology (including two years Marie Curie fellowship). Since 2003 he works in San Sebastián, holding scientific positions at Donostia International Physics Center and Centro de Física de Materiales CSIC-UPV/EHU.

His research interests focus on the atomistic simulations of structural, optical and magnetic properties of solids and nanostructures, such as graphene and 2D materials, nanotubes, alloys, layered oxides and cements. He published over 120 peer-reviewed papers in such journals like Physical Review Letters, Applied Physics Reviews, Advanced Materials, Nano Letters, Nanoscale, Nanophotonics, 2D Materials, Chemistry of Materials, Cement and Concrete Research, Carbon and Acta Materialia (H-index = 38).

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