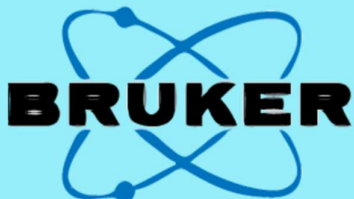




Young Researchers Retreat 2022

Participants & their science

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Alejandro Yeste Vazquez – PhD student at Vrije Universiteit Amsterdam – Structural biology
Cyclic peptides as inhibitors of oncogenic Wnt signalling

My name is Alejandro I'm from Barcelona and I'm doing my PhD in Amsterdam since 2020, working in Prof. Grossmann group. I'm currently working in two different projects although the goal is the same for both, that is the design and synthesis of peptides able to target a protein-protein interaction of interest. Both projects aim to target proteins related to the initiation or progression of certain types of cancer and to do that I express and purify all the target proteins and binders; I synthesize the peptides and do the first biophysical assays to proof or not the binding. In some previous research in my group crystallography has been used as part of the process, as I will talk later, and to what concern my workflow, crystallography just started now.

On my free time I really like to go out with friends and partying time to time, as well as travel as much as I can even for short times.

Canan Durukan – PhD student at Vrije Universiteit Amsterdam – Structural biology
Peptidomimetic-Fragment Conjugates for NF-YB/C modulation

My name is Canan Durukan, right after obtaining my master's degree in Chemistry as well as my bachelor's degree in Istanbul, Turkey, I started my PhD in Sven's Lab at VU Amsterdam in summer 2020. My research focus is on bimolecular interactions and their modifications, specifically for protein-protein interaction modifications of NF-Y transcription factor. The major part of my work so far was the study of proteins and ligand binding. It is both interesting and fun to carry out research about proteins and discover this complex world of proteins and crystallography.

Ida de Vries – PhD student at the Netherlands Cancer Institute – Structural biology
AlphaFill: Enriching AlphaFold models with ligands, co-factors and metal ions

Trained as a medicinal chemist with an extraordinary interest in computational drug design, I am currently working with Robbie Joosten at the NKI. With our PDB-REDO pipeline we aim for an automated method that rebuilds, re-refines and optimizes macromolecular structures obtained with X-ray crystallography in an uniform and FAIR (findable, accessible, interoperable, reproducible) manner. I have been working on optimizing the validation for nucleic acids and hope to improve how our pipeline deals with small molecules in the future. Currently, my main focus is to implement a functionality for processing and analyzing all data that is obtained in fragment screening campaigns. Additionally, motivated by the availability of protein predictions through the AlphaFold database, I have been working on AlphaFill. Herein, we enrich the AlphaFold models with ligands, co-factors and metal ions to provide a new tool and database that scientists can use in designing their experiments.

In my spare time I like to bake and cook (still some experimental chemistry), or go for a hike.

Jitse van der Horn – PhD student at Utrecht University - Structural biology
Diffuse Scattering in Protein X-Ray Crystallography

My name is Jitse. I am from Heerenveen, and I moved to Utrecht in 2012 to do my bachelor's in chemistry. I enjoyed this so much, that I also decided to do my master's there. One thing led to another, and currently I am doing a PhD in protein crystallography with Loes Kroon-Batenburg at Utrecht University. Protein structures obtained through X-ray crystallography represent an average conformation of all protein molecules in a crystal. In reality, proteins are very flexible and dynamic. Even in a crystal, they can adopt many different conformations. Clues about their disorder can be captured during X-ray diffraction experiments, in the form of diffuse scattering. Here, we model experimentally observed diffuse scattering by simulating correlated motions inside a supercell.

Sandra Eltschkner – PostDoc at University of Amsterdam – Structural biology
Hijacking the plant DNA replication machinery - towards the structure of the viral replication initiator protein and its interaction partners

I am a postdoc at the Molecular Plant Pathology group at the UvA, and I have broad experience in applying molecular structural biology to many different systems across the kingdoms of life. Currently, I am investigating how plant viruses exploit the host replication machinery to promote infection. I believe that food security in the face of a growing population and climate change will be a major challenge in the years to come.

Problems with begomoviruses have been heavily aggravated in recent years; particularly Tomato Yellow Leaf Curl Virus (TYLCV) causes severe damage on tomato and cucurbits impacting growers worldwide. Climate change has allowed the main vector for viral transmission, the whitefly *Bemisia tabaci*, to massively populate more moderate climate zones including the Mediterranean. With the ban of pesticides and a lack of strong resistance genes in our crops, we urgently need alternative strategies to halt viral spread. Begomoviruses rely heavily on host factors for their genome replication. The viral proteins need to reprogram the host cell cycle and recruit the plant DNA-replication machinery to the viral DNA. Only one viral protein, the Replication initiator protein (Rep), is essential and sufficient to promote viral DNA replication inside plant cells. Our goal is to elucidate the structure of Rep in complex with PCNA, a central processivity factor for DNA polymerases, to gain insight in how Rep orchestrates DNA replication.

Wouter Beugelink – PhD student at Utrecht University – Structural biology
Solution scattering of the Teneurin ectodomain reveals compact conformation

I am Wouter, an aspiring structural biologist working as a PhD student in the Janssen lab at Utrecht University. I combine cryo-electron microscopy with crystallography and solution scattering to study neuronal receptors and their ligands.

Albaraa Falodah – PhD student at Utrecht University – Material science
MetaChemistry: the way to the Philosopher's Stone?

At the start of my journey into Chemistry. Currently learning different spectroscopic techniques to research polymer catalysis on a level between the fundamental and the industrial.

Essentially, I'm passionate about "The New Chemistry" – integrating knowledge from different branches back into a holistic system beyond disciplines. I believe this is the only way for humanity to flourish on this beautiful planet.

Jyoti Yadav – PhD student at Technobis Crystallization Systems - Material Science
Effect of solvent composition on solubility, thermodynamics, MSZW and crystal habit of ascorbic acid

I am pursuing my Ph.D. from Indian Institute of Technology (IIT), Ropar, India, in the field of Crystallization. I moved to the Netherlands after my marriage and currently doing an internship at Technobis Crystallization Systems, Alkmaar, The Netherlands. I did my bachelor's and Master's in chemical engineering from India.

For my PhD thesis, I am working on ascorbic acid (Vitamin C), which has applications in pharmaceutical, agriculture, health, and personal care industries. The research focus on studying the effect of solvent composition on solubilities, Metastable zone with, thermodynamic properties and crystal habit of ascorbic acid.

Lian Blijelevens – PhD student at Radboud University – Material science
Screening of double sulfate salts for heat storage Mat4Heat: Heat batteries for sustainability

I am a crystal scientist at the department of Solid State chemistry at Institute of Molecules and Materials of the Radboud University. I am in the last year of my PhD where I have been researching heat storage in salt hydrates. I have previously researched the effect of additives on NaCl and paracetamol. I love crystals due to their beautiful symmetries and colors (sometimes induced by polarization). In relation to that I most appreciate research techniques which actually visualize what you are researching so both optical and electron microscopic techniques. Furthermore, I really appreciate the symmetries in Islamic architecture, especially after learning they already used the "forbidden" 5-fold symmetries in their tiling's centuries before we discovered the existence of quasicrystals. Finally, I am interested in diversity and inclusion.

**Shilpa Ramesh – PhD student at Maastricht University – Material science
Prussian Blue Analogues**

I am Shilpa Ramesh from Mumbai, India. I did my Master's at Amity University, Delhi in Applied Chemistry and I am doing my PhD at Circular Chemical Engineering, Maastricht University on the topic Electrolyte materials using colligative properties. I am working on Battery materials presently. I have specialized experience in spectroscopy and a bit of electrochemistry.

Simon Lepinay – PhD student at University of Amsterdam – Material science

TBA

**Tadeus Hogenelst – PhD student at University of Amsterdam & ARCNL - Material Science
PLD growth of (TaNbHfTiZr)C multi-elemental carbide: influence of deposition pressure and
substrate temperature on crystallinity**

Hey, I'm Tade. I work in applied physics and my research interests are centred around materials synthesis. Current projects that I work regard the growth of multi-elemental ceramic thin films. I use various methods to grow and evaluate chemical and structural information of the materials in question. Furthermore, some of the films may be of interest in application, and hence, there is an interest in characterizing material properties of the as-grown films. Other research interests concern the application of ball milling synthesis for alloy formation. My talk will be about growth of (TaNbHfTiZr)C multi-elemental carbide, in which I will zoom in on the influence of deposition pressure and substrate temperature on the crystallinity of the films. I will consider XPS and grazing-incidence XRD data to identify surface composition and structure.

Besides my research interests, I have a strong interest in music and making music. I'm a drummer, and next to acoustic percussion, I also synthesize electronic music. I furthermore enjoy good food and I practice martial arts.

**Zixiong Sun - Postdoc at University of Twente - Material Science
Optimizing the energy storage performances of ferroelectric multilayers by fabricating Schottky
barrier**

Dr. Zixiong Sun, who is from the University of Twente, with a h-index of 12 according to the *wos* database, has a long time research background of ferroelectric oxide thin films, especially for ferroelectric/piezoelectric-related materials. Dr. Zixiong Sun has a very deep work for fabricating ferroelectric multilayers for ferroelectric energy storage capacitors. Currently, by some latest work about the ferroelectric semiconductor/memristor in UT, he proposed a fancy strategy for enhancing the energy storage density of ferroelectric capacitors by fabricating the Schottky barrier. It is quite different from the common method for increasing the ferroelectric energy storage performances by simply increasing the electrical breakdown strength or polarization. It can be considered as optimizing the first quartile of P-E loop at the expense of the third quartile, which is actually not necessary for energy storage properties.