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SUSTAINABILITY AND CIRCULARITY OF TRANSPARENT WOOD: THE ROLE OF THE *AI-TRANSPWOOD* PROJECT IN HIGHLIGHTING THE POTENTIAL OF THIS NEW MATERIAL

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Introduction

The current challenge toward the development of more sustainable processes and the design of low environmental impact and efficient materials is having a significant impact on the academic and industrial communities. In this context, the design, implementation, and application of novel polymer-based systems that can directly be obtained from available biomasses (without impacting other supply chains, like the food-related ones), by using "green" technologies is currently becoming necessary and demanding, also for fulfilling the circular economy concept [1].
The latter is perfectly matched by wood, a renewable and recyclable biomass that has massively been employed by mankind over the centuries. Wood is a natural composite material with unique mechanical, thermal, and environmental properties, which make it appropriate for several applications dealing with civil engineering, art, household uses, and business uses (including furniture, stationery, shipbuilding, and fuel) [2].
Nonetheless, wood exhibits a complex hierarchical structure that accounts for a high anisotropy, due to the presence of open channels aligned in the growth direction, and a peculiar micro-, meso-, and macro-porosity. As a result, it is an opaque material in which the lignin (one of the three main constituents together with cellulose and hemicellulose) favors the occurrence of light-scattering phenomena [3]. Though the idea of making wood a transparent material ("Transparent Wood", TW) dates to 1992 [4], it was rediscovered and implemented only during the last fifteen years [5]. Besides, it is now possible to provide TW not only with high optical transmittance but also with other characteristics comprising environmental protection, flame retardance, photoluminescence, and energy storage capability, among others.
As a consequence, at present TW is reasonably considered a novel, green, and smart "building block", suitable for the design of both structural and functional systems to be exploited in such key-performing sectors as optoelectronics, photovoltaics, buildings, furniture, and automotive.

The making of Transparent Wood

Lignin removal and lignin modification are the two possible ways to produce Transparent Wood. The former is carried out by exploiting specific chemical processes (alkali or acidic treatments, $NaClO_2$ bleaching, H_2O_2 treatments): this way it is possible to almost completely remove the lignin (the residual lignin is below 0.8-1 wt.%) [6]. However, lignin removal exerts a detrimental effect on the overall mechanical behavior of wood and often requires the use or the formation of toxic substances (including sulfides or chlorine-containing compounds): these issues can be solved by altering lignin, and, in particular, by removing or modifying only its chromophoric groups [7].
After delignification, the micro-, meso-, and macro-porous Transparent Wood is ready to be modified/functionalized according to the envisaged uses. The currently employed methods involve the infill of the lumen (i.e., of the cavity of a wood cell where free water is held), the modification of the cell wall, or the modification of the interface between the cell wall and lumen. For this purpose, it is usual to carry on physical sorption processes, promote the *in situ* precipitation of metal or inorganic particles from the corresponding salt solutions, or perform chemical reactions with reactive monomers, with which wood pores and cavities have been previously impregnated, or thermally treat the wood's main components,

aiming at promoting phase separation phenomena [8].

The AI-TranspWood project

AI-TranspWood project [9] was funded by the European Commission under the call HORIZON-CL4-2023 -RESILIENCE-01-23 – "Computational models for the development of safe and sustainable by design chemicals and materials". It started on January 1, 2024, and will end on December 31, 2026.
The project's ambition is to create an AI (Artificial Intelligence)-driven multiscale methodology for new Safe and Sustainable by Design, and functional wood-based composites and demonstrate the concept for TW. This way, it will be possible to elaborate a consistent and reliable computational framework, assisted by physics-based computational models, AI and Machine Learning (ML) tools, able to predict and optimize the properties exhibited by Transparent Wood, based on the type of wood and its specific modification/functionalization.
The project focuses on four main objectives, namely:

- to create an AI-driven multiscale methodology for TW and functional wood-based composites, also using the Safe and Sustainable by Design approach
- to develop multiscale models from the atomistic scale to continuum for the manufacturing process and the mechanics of the Transparent Wood
- to openly share the developed computational models within the European Environment for Scientific Software Installation (EESSI, https://www.eessi-hpc.org/)
- to make user-friendly surrogate models also available in the VTT Modeling Factory environment (modellingfactory.org), along with an LCA tool, for industrial use
- to perform TW demo cases, aiming at its subsequent commercialization in the construction, automotive, electronics, and furniture industries.

The project involves 13 partners (academic and industrial) from 10 countries.
As shown in Figure 1, the project activities are organized according to 17 workpackages (WPs), which encompass the development and experimental validation of robust and reliable molecular, multiscale, and process models, as well as the envisaged management, dissemination, communication, and exploitation activities.

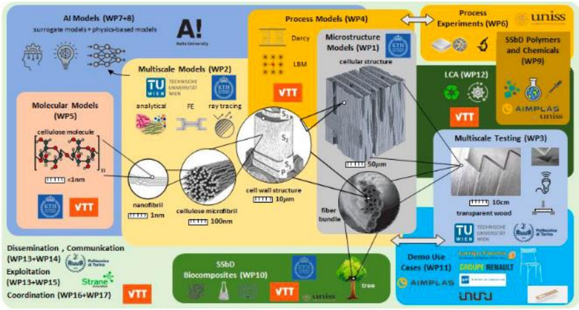

Figure 1: The structure of the AI-TranspWood project.

AI-TranspWood proposes a systematic approach involving three stages for complementing the physics-based modeling with AI and ML tools, as shown in Figure 2.

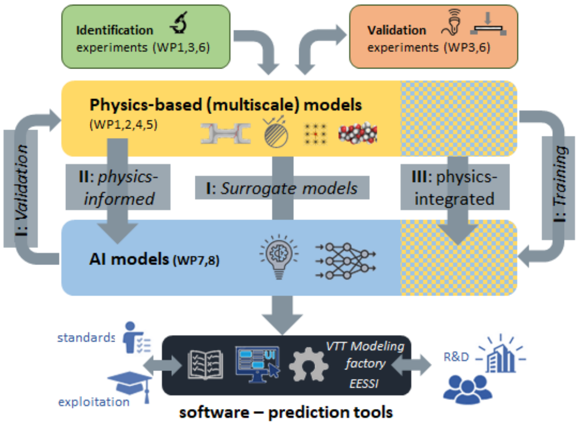

Figure 2: Conceptual three-stage process to link physics-based models to AI methodology, and model classes that will then be implemented in the predictive software.

All these activities will hopefully widen the knowledge about TW and its big potential in materials science and technology, making all the interested people (stakeholders, end users, etc.) aware of its existence, availability, and exploitability.

Acknowledgments

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