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By accepting these Terms of Use, the user enters into an agreement with NanoCrystal made up by the contents of these Terms, in order to regulate the user's access and use of the NanoCrystal. Users which accept these Terms of Use hereby represent and warrant that:

They accept to be bound by these Terms of Use, either individually, or in representation of an organisation;

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Their use of the NanoCrystal will be carried out in accordance with all applicable laws and regulations;

In case users publish results produced from NanoCrystal or using NanoCrystal by any means, they are obligated to cite:

Chatzigoulas, A., Karathanou, K., Dellis, D., & Cournia, Z. (2018). NanoCrystal: A Web-Based Crystallographic Tool for the Construction of Nanoparticles Based on Their Crystal Habit. Journal of Chemical Information and Modeling, 58(12), 2380-2386

In the event of doubts concerning the Terms of Use, NanoCrystal may be contacted at: zcournia@bioacademy.gr or chatzig@di.uoa.gr.

For information on the processing of personal data on users which is carried out via the NanoCrystal, please see the NanoCrystal privacy policy.

1. Services provided

NanoCrystal creates nanoparticle models from any crystal structure guided by their preferred equilibrium shape in standard conditions (crystal habit), our algorithm uses input from quantum mechanical calculations based on the Wulff construction. The Wulff construction employs energy minimization arguments to demonstrate that certain crystal planes are preferred over others, with their distance from the origin being proportional to their surface energy. The input parameters for determining this equilibrium nanoparticle structure are the preferred growing planes as Miller indices, the energy of each plane, and the desired size of the nanoparticle. Additionally, NanoCrystal has the option to keep the stoichiometry of the system and/or to create spherical nanoparticles. As an output, the user can retrieve the atom coordinates of the produced nanoparticle in .pdb and .xyz formats.

2. Copyright / Intellectual Property

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3. Membership or subscription fees

NanoCrystal is free for every user and no registration is required.

4. User data protection

The output of NanoCrystal belongs to the users and we have no authority to use these results for our own benefit or to share them with others. The output link and output data are kept for 2 (two) days and then they are automatically deleted.

5. Liability

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