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Πλατφόρμα δημοσιεύσεων Ανοικτής Πρόσβασης

2021

Χαρά Ράμμα

Βιβλιοθήκη Νομικής Σχολής

ΕΛΛΗΝΙΚΗ ΔΗΜΟΚΡΑΤΙΑ
Εθνικόν και Καποδιστριακόν Πανεπιστήμιον Αθηνών
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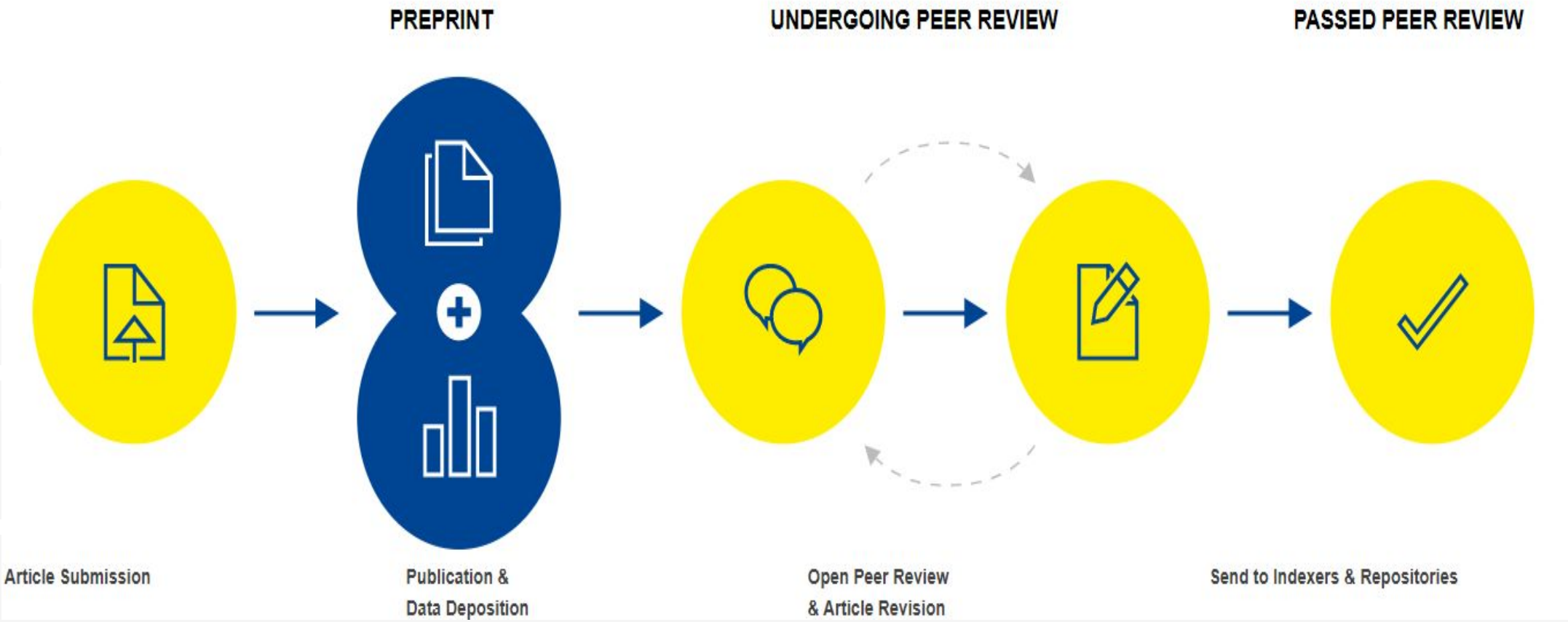

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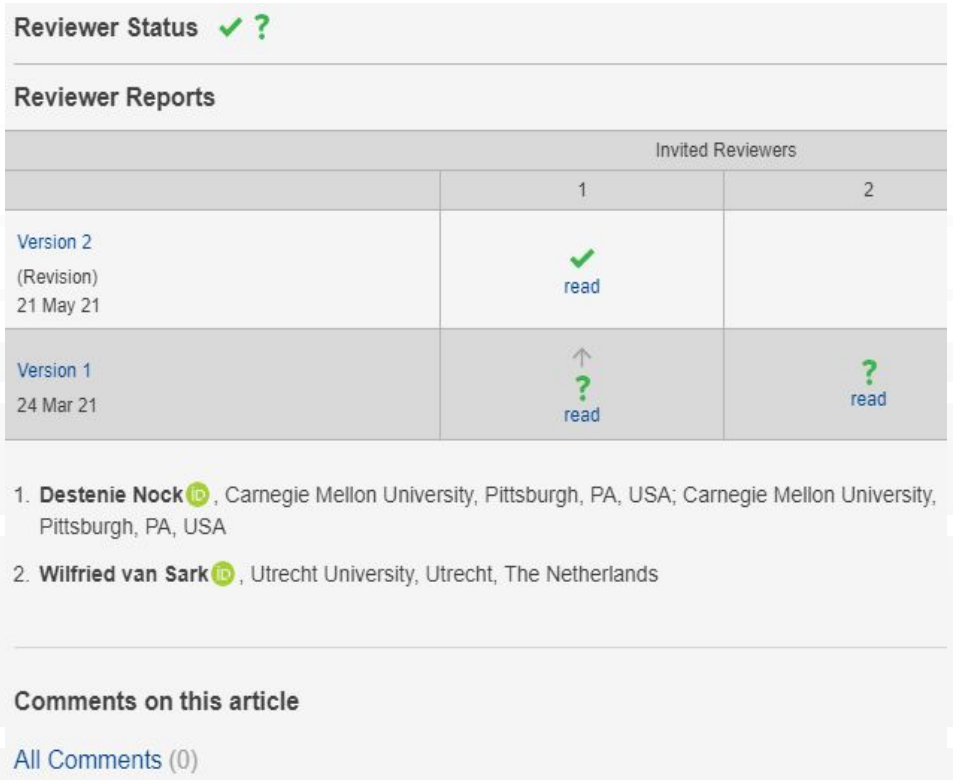

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SOFTWARE TOOL ARTICLE

REVISED The abTEM code: transmission electron microscopy from first principles [version 2; peer review: 2 approved]

Jacob Madsen, Toma Susi

REVISED **Amendments from Version 1**

All reviewer comments have been addressed. Updates to the code include: interpolation with Fourier-space padding, corrections to use case examples (including improved line styling to accommodate impaired color vision), and added repository examples including PACBED and partial coherence in 4D-STEM.

See the detailed response from the author(s) to the review by Hamish Brown
See the detailed response from the author(s) to the review by Colin Ophus

1 Introduction

Transmission electron microscopy (TEM) is one of the most versatile and powerful experimental tools for the imaging and diffraction of structures ranging from the micrometer scale with sub-Ångström resolution now routinely achievable in modern aberration corrected instruments. In TEM, information about the sample structure is encoded in the scattering of the electron waves by the full electromagnetic potential of the specimen, which is dominated by the atomic electrostatic potentials. These potentials include the contribution of the screened nuclear cores as well as the valence electron density of the sample, and since valence electrons are responsible for binding the material together, studying them is of significant scientific interest.

The modern electron microscope should be an ideal tool for the high-resolution imaging of charge redistribution caused by chemical bonding, but these measurements are a challenge because only a small fraction of the total electrons in a material participate in bonding, and because the dense cores dominate the scattering signal. However, as improvements in instrumentation and techniques continue rapidly, this is likely to increasingly change, as evidenced by the surging popularity of techniques such as four-dimensional scanning transmission electron microscopy (4D-STEM) combined with ptychography in materials science, and cryogenic microcrystal electron diffraction in structural biology.

To reliably quantify subtle differences in the scattering signal, precise alignment of the instrument and a careful comparison between theoretical models and experiments are required. The use of image simulations has long aided this process, and many excellent codes have been developed. However, these have exclusively relied on the independent atom model (IAM), which approximates the specimen potential as a superposition of isolated atoms, completely neglecting chemical bonding. A growing number of studies are going beyond the IAM by calculating the potential using density functional theory (DFT)[1–7]. As expected, these studies find a better agreement for a range of different materials when comparing to measurements that are sensitive to valence electron density, such as holography and various forms of phase-contrast imaging.

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Responses (1)

AUTHOR RESPONSE 2 MAY 2021

Toma Susi
University of Vienna, Vienna, Austria

Original comments by the reviewer are reproduced in *italics* below, followed by our point-by-point replies.

The field of TEM image simulation is now very mature with many free and open source simulation codes available. However many of these codes are written in low-level languages such as Fortran and C++ which means that they can be inflexible and difficult to modify, especially for the average microscop...

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1) Open Research Europe. (2021). https://open-research-europe.ec.europa.eu/

2) Τσουκαλά, Β. (2021). *Open Research Europe: The European Commission Open Access Publishing Platform* [Webinar]. https://www.youtube.com/watch?v=yCjg6vjnpNU&ab_channel=OpenAIRE_eu