

**Anisotropic percolating pathways in the thin films of polymeric PEDT/PSS complex and their relation to the electrical conductivity as revealed by the mesoscale simulation**

Kaevand, Toomas; Kalda, Jaan; Öpik, Andres; Lille, Ülo Technological developments in networking, education and automation 2010 / p. 263-268

**Atomistic molecular simulation of thermal volume expansion of Estonian kukersite kerogen**

Kaevand, Toomas; Lille, Ülo Oil shale 2005 / 3, p. 291-303 : ill [https://artiklid.elnet.ee/record=b2349330\\*est](https://artiklid.elnet.ee/record=b2349330*est)

**Correlated percolating networks in the thin film of polymeric PEDT/PSS complex as revealed by the mesoscale simulation**

Kaevand, Toomas; Kalda, Jaan; Öpik, Andres; Lille, Ülo Macromolecules 2009 / 4, p. 1407-1409 : ill  
<https://pubs.acs.org/doi/abs/10.1021/ma802160x>

**Correlation of the morphology and electrical conductivity in thin films of PEDT/PSS complex: an integrated meso-scale simulation study**

Kaevand, Toomas; Kalda, Jaan; Kukk, Vello; Öpik, Andres; Lille, Ülo Molecular simulation 2011 / p. 495-502 : ill  
<https://www.tandfonline.com/doi/abs/10.1080/08927022.2011.554549>

**ETAIS2 ühendab võimsad arvutuskeskused teaduspilveks**

Kaevand, Toomas Mente et Manu 2017 / lk. 20-21 : fot [https://www.ttu.ee/public/m/mente-et-manu/MM\\_03\\_2017/mobile/index.html#p=1](https://www.ttu.ee/public/m/mente-et-manu/MM_03_2017/mobile/index.html#p=1)

**From the molecules of resorcinolic lipids to alga G. prisca globular colonies in kukersite microfossils : a multiscale simulation study**

Kaevand, Toomas; Lille, Ülo Oil shale 2020 / p. 281-287 : ill <https://doi.org/10.3176/oil.2020.4.02> Journal metrics at Scopus Article at Scopus Journal metrics at WOS Article at WOS

**Interaction of Estonian kukersite with organic solvents : a volumetric swelling and molecular simulation study**

Savest, Natalja; Oja, Vahur; Kaevand, Toomas; Lille, Ülo Fuel 2007 / 1/2, p. 17-21

**Lipase-catalysed acyl transfer in deoxysugars : a computational study**

Kaevand, Toomas; Villo, Ly; Metsala, Andrus; Parve, Omar; Lille, Ülo International journal of engineering and applied sciences (EAAS) 2015 / p. 1-7 : ill

**A mesoscale simulation of the morphology of the PEDT/PSS complex in the water dispersion and thin film : the use of the MesoDyn simulation code**

Kaevand, Toomas; Öpik, Andres; Lille, Ülo Advances in computer and information Science and Engineering. XVIII 2008 / p. 540-546 : ill

**On the charge carrier time-of-flight mobility and the ordering effects in the microcrystalline PEDOT/PSS complex : a morphology-based simulation study**

Kaevand, Toomas; Kalda, Jaan; Lille, Ülo International journal of renewable energy and biofuels 2013 / p. 1-13 : ill

**On the percolation behavior of the thin films of the PEDT/PSS complex : a mesoscale simulation study**

Kaevand, Toomas; Kalda, Jaan; Öpik, Andres; Lille, Ülo Technological Developments in Education and Automation 2010 / p. 103-107 : ill

**Resorcinolic lipids as an essential source material of kukersite kerogen**

Lille, Ülo; Kaevand, Toomas International Symposium "Oil shale 100 years" : Estonia, Sept. 20-23, 2016 : [abstracts] 2016 / p. 53-54