

# **VII Workshop on Electron-Volt Neutron Spectroscopy 2017**

Journal of Physics: Conference Series  
Volume 1055

Rome, Italy  
7 - 8 November 2017

## **Editors:**

**G. Romanelli**

**G. Festa**

**M. Krzystyniak**

**C. Andreani**

**F. Fernandez-Alonso**

**R. Senesi**

ISBN: 978-1-5108-6792-5

ISSN: 1742-6588

**Printed from e-media with permission by:**

Curran Associates, Inc.  
57 Morehouse Lane  
Red Hook, NY 12571



**Some format issues inherent in the e-media version may also appear in this print version.**

Copyright© (2017) by the Institute of Physics  
All rights reserved. The material featured in this book is subject to  
IOP copyright protection, unless otherwise indicated.

Printed by Curran Associates, Inc. (2018)

For permission requests, please contact the Institute of Physics  
at the address below.

Institute of Physics  
Dirac House, Temple Back  
Bristol BS1 6BE UK

Phone: 44 1 17 929 7481  
Fax: 44 1 17 920 0979

[techtracking@iop.org](mailto:techtracking@iop.org)

**Additional copies of this publication are available from:**

Curran Associates, Inc.  
57 Morehouse Lane  
Red Hook, NY 12571 USA  
Phone: 845-758-0400  
Fax: 845-758-2633  
Email: [curran@proceedings.com](mailto:curran@proceedings.com)  
Web: [www.proceedings.com](http://www.proceedings.com)

# Table of contents

## Volume 1055

### **VII International Workshop on Electron-Volt Neutron Spectroscopy**

**7–8 November 2017, Rome, Italy**

**Accepted papers received: 3 July 2018**

**Published online: 17 July 2018**

### **Preface**

[Neutrons matter: VII international workshop on electron-Volt neutron spectroscopy – A preface to the workshop proceedings](#)

G Romanelli, G Festa, M Krzystyniak, C Andreani, F Fernandez-Alonso and R Senesi

[Peer review statement](#)

### **Papers**

#### **The science**

[Observation of the stretch mode in H<sub>2</sub> and D<sub>2</sub> by inelastic neutron scattering spectroscopy](#)

S F Parker, R A Ewings, F Fernandez-Alonso and D Colognesi.....1

[Inelastic and deep inelastic neutron spectroscopy of water molecules under ultra-confinement](#)

A I Kolesnikov, G F Reiter, T R Prisk, M Krzystyniak, G Romanelli, D J Wesolowski and L M Anovitz.....8

[Hydrogen dynamics in solid formic acid: insights from simulations with quantum colored-noise thermostats](#)

K Drużbicki, M Krzystyniak, D Hollas, V Kapil, P Slavíček, G Romanelli and F Fernandez-Alonso.....19

Mass-selective neutron spectroscopy of glassy versus polycrystalline structures in binary mixtures of beryllium and zirconium

M Krzstyniak, G Syrykh, A Stolyarov, R A Sadykov, J Armstrong, I da Silva, G Romanelli and F Fernandez-Alonso.....38

Neutron resonance capture analysis and chemometric tools: an integrated approach

M Nardini, C Andreani, R Senesi, A Scherillo, F D'Agostino, L Romano, C Scatigno and G Festa.....52

Nitrogen doping and the performance of superconducting radio-frequency niobium cavities: insights from neutron diffraction and neutron Compton scattering

M Krzstyniak, M J Gutmann, G Romanelli, Y Trenikhina, A Romanenko and F Fernandez-Alonso.....59

Fractal dimension as a scaling law for nuclear quantum effects: a neutron Compton scattering study on carbon allotropes

J Armstrong, M Krzstyniak, G Romanelli, S F Parker, K Družbicki and F Fernandez-Alonso.....69

**The method**

Enhancement of counting statistics and noise reduction in the forward-scattering detectors on the VESUVIO spectrometer

P Ulpiani, G Romanelli, L Arcidiacono, D Onorati, G Festa, M Krzstyniak, E Schooneveld, F Fernandez-Alonso, C Andreani and R Senesi.....94

Gamma background characterization on VESUVIO: before and after the moderator upgrade

D Onorati, C Andreani, L Arcidiacono, F Fernandez-Alonso, G Festa, M Krzstyniak, G Romanelli, P Ulpiani and R Senesi.....101

Absolute efficiency calibration of a coaxial HPGe detector for quantitative PGAA and T-PGAA

A Parmentier, L Arcidiacono, R Senesi, G Romanelli, C Andreani, J Moir and G Festa.....108

Nuclear kinetic energies from final-state effects in the harmonic limit

M Krzystyniak, G Romanelli, R Tolchenov, M Gigg, B Hewer and F Fernandez-Alonso.....118

Model selection in neutron Compton scattering - a Bayesian approach with physical constraints

M Krzystyniak, G Romanelli, K Drużbicki, R Tolchenov, M Gigg, B Hewer and F Fernandez-Alonso.....133

Procedure for the determination of effective temperatures employing VESUVIO spectrometer

J Dawidowski, L A Rodríguez Palomino, G Romanelli and M Krzystyniak.....150

A McStas simulation of the incident neutron beam on the VESUVIO spectrometer

A Di Giulio, M Zanetti, G Romanelli, M Krzystyniak, R Senesi and F Fernandez-Alonso.....166

Neutron-resonance capture analysis on the VESUVIO spectrometer: Towards high-throughput material characterisation

G Romanelli, M Krzystyniak and F Fernandez-Alonso.....173

Data analysis of neutron Compton scattering experiments using MANTID

G Romanelli, B Hewer, M Krzystyniak, M Gigg, R Tolchenov, S Mukhopadhyay and F Fernandez-Alonso.....183

## **Conclusions**

The road to a station for epithermal and thermal neutron analysis

G Romanelli, M Krzstyniak, G Festa, C Andreani, F Fernandez-Alonso and R Senesi.....201