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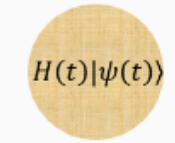

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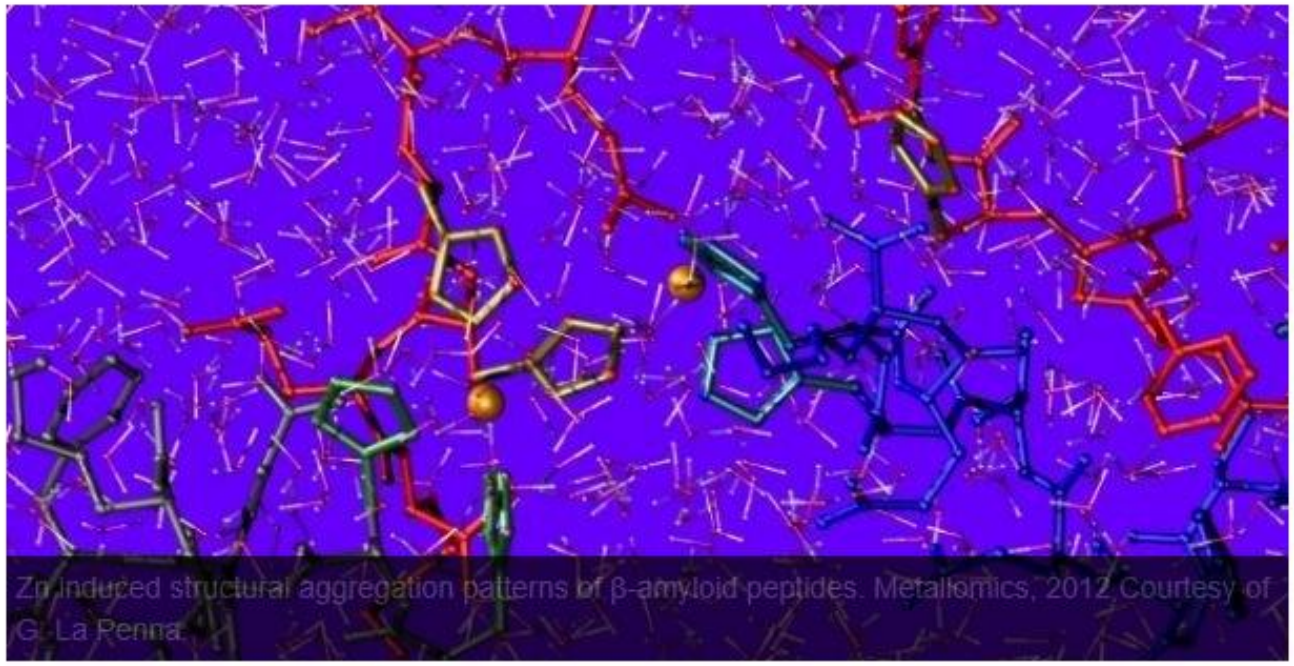

Zn induced structural aggregation patterns of β-amyloid peptides. Metallomics, 2012 Courtesy of G. La Penna.

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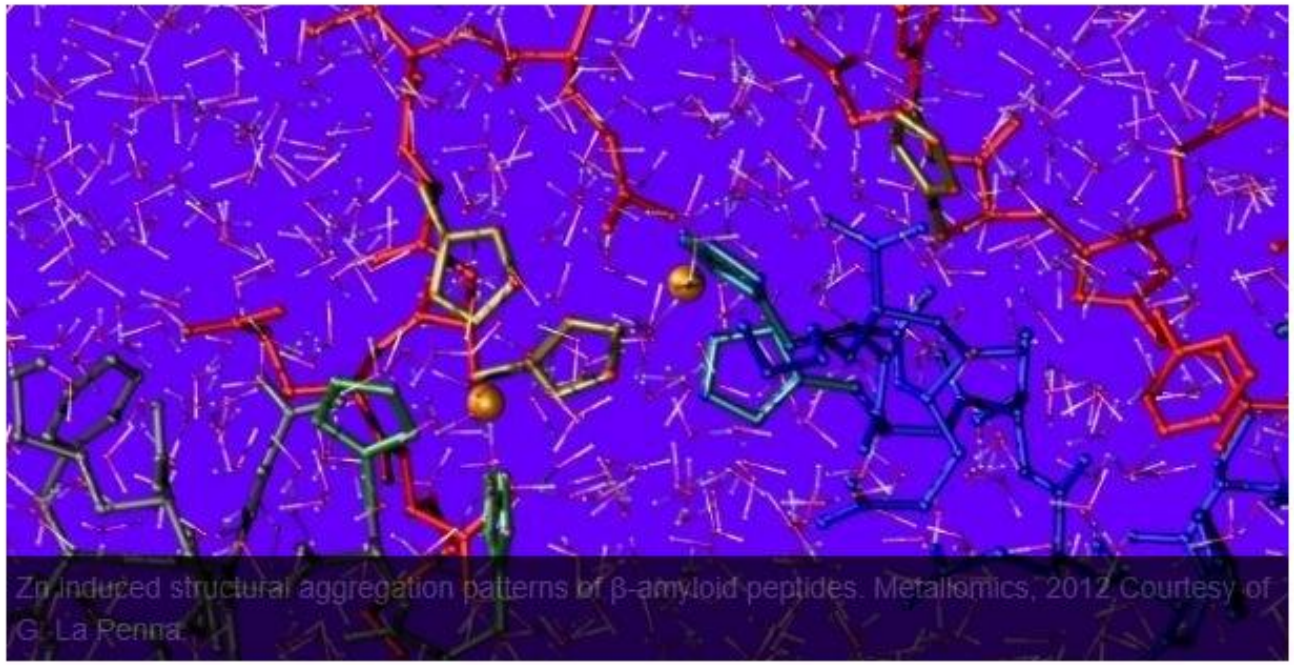

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How to cite?

QUANTUM ESPRESSO is an Open Source distribution. We shall greatly appreciate if scientific work done using QUANTUM ESPRESSO will contain an explicit acknowledgement and the following references:

P. Giannozzi *et al.*, J.Phys.:Condens.Matter **21**, 395502 (2009) http://dx.doi.org/10.1088/0953-8984/21/39/395502

P. Giannozzi *et al.*, J.Phys.:Condens.Matter **29**, 465901 (2017) http://iopscience.iop.org/article/10.1088/1361-648X/aa8f79

(Full reference, BibTeX format). Please also see the user documentation of each specific package for further recommended citations.

How to download?

QUANTUM ESPRESSO is currently distributed as source packages, but selected binary packages for Linux, Mac-OS and Windows are also available. The current stable version can be downloaded from:

- GitHub (recommended), or alternatively from
- GitLab (click on the "cloud with a down arrow" to download).

Download

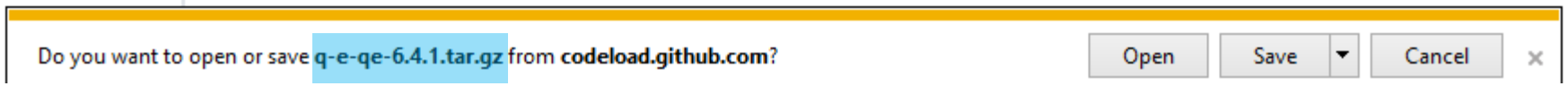
https://github.com/QEF/q-e/releases

Problems fixed in 6.4.1 branch :

- Two bugs fixed in HP: 1) the code was not working correctly when fractional translations were present, 2) there was a bug in the case when either there is only one k point, or when k pools are used and some of the pools have only one k point.
- Restart of ph.x with 2D boundary conditions has been fixed (see gitlab issue #102)
- XML file correctly written if tetrahedra are used (see gitlab issue #103)

▼ Assets 5

backports-6.4.1.diff	25.4 KB
patch_old_intel_to_6.4.1	16.6 KB
qe-6.4.1_release_pack.tgz	80.3 MB
Source code (zip)	
Source code (tar.gz)	



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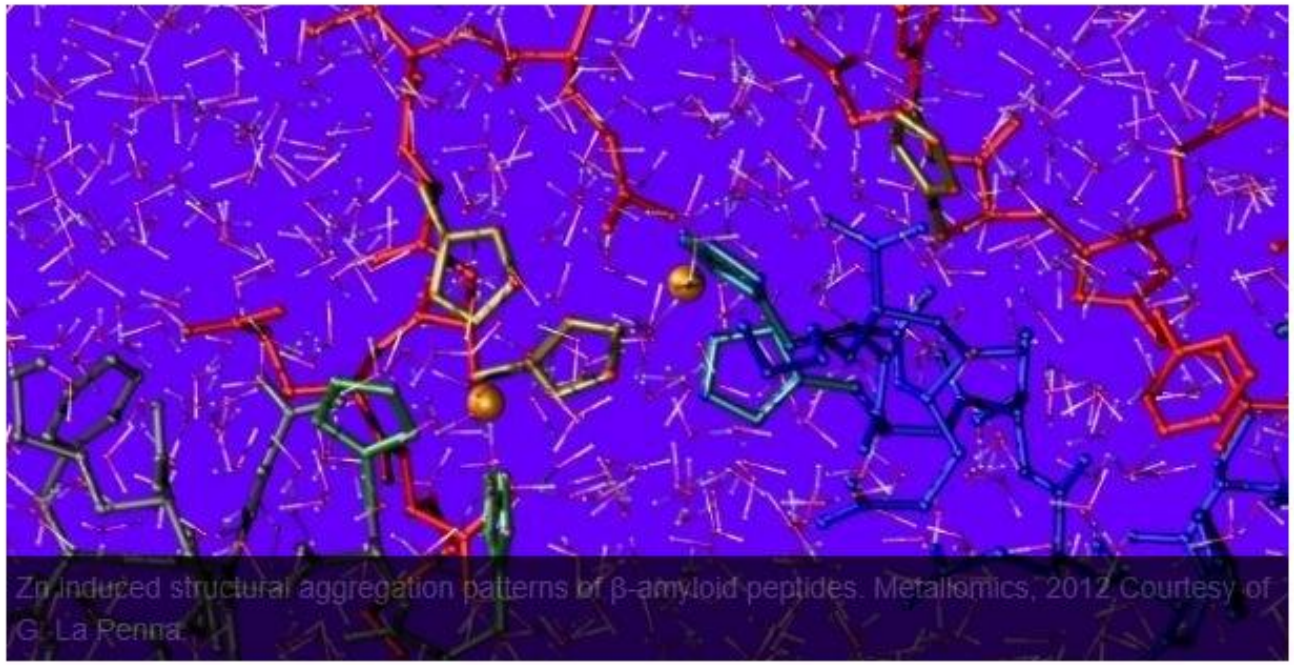

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Hartwigesen-Goedecker-Hutter PP table
Old FHI PP table

PSLIBRARY

Ready-to-use pseudopotentials from PSlibrary (*recommended*). For other ready-to-use tables, follow the links of the menu at the left. For more info, see here.

1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca		21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr		39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57-70 *	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89-102 **	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt									

* Lanthanoids	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb
** Actinoids	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No

Some useful resources

- Official quantum espresso website
- https://www.quantum-espresso.org/

- Other important resources
  - Documentation https://www.quantum-espresso.org/resources/users-manual
  - Examples offered by the software
  - Pseudopotentials:
    - Official site: https://www.quantum-espresso.org/pseudopotentials
    - SSSP: https://www.materialscloud.org/discover/sssp/table/efficiency
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