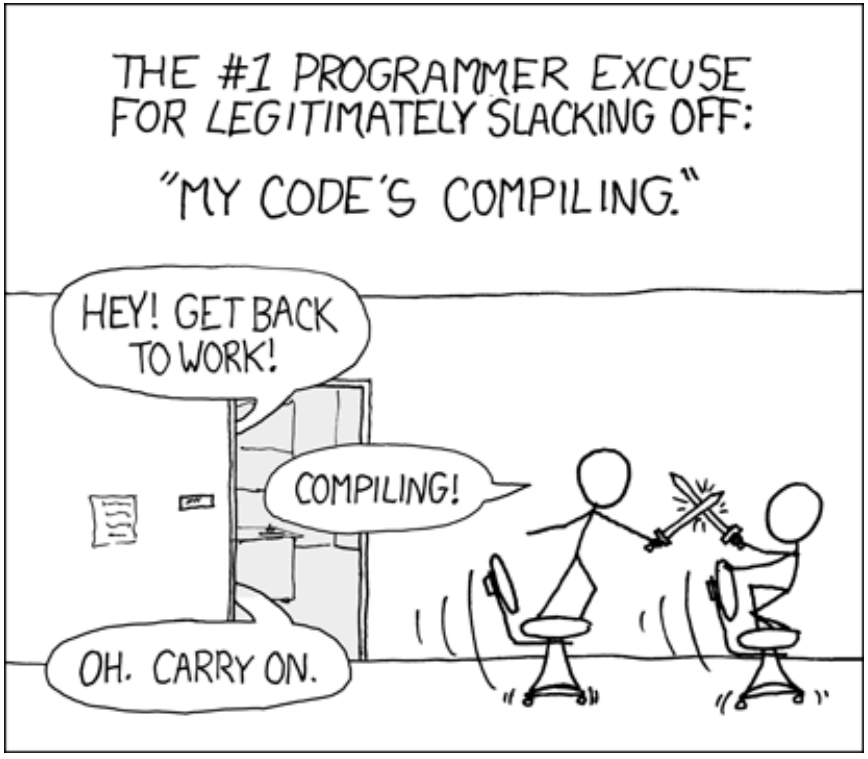
RCS RESEARCH COMPUTING SERVICE
Gateway to Discovery

Scientific Reproducibility:

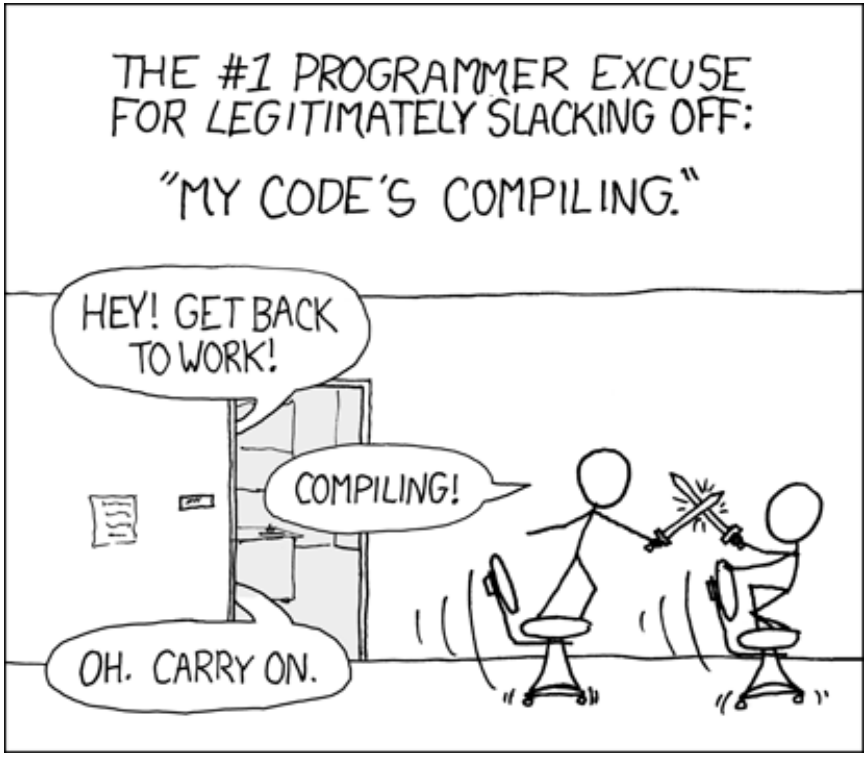
The importance of reliable and sustainable software installation.

Jörg Saßmannshausen



Source: https://xkcd.com/303/

Whoami?



Source: https://xkcd.com/303/

ACS OMEGA

http://pubs.acs.org/journal/acsodf

Article

Detailed Density Functional Theory Study of the Cationic Zirconocene Compound $[Cp(C_5H_4CMe_2C_6H_4F)ZrMe]^+$

Jörg Saßmannshausen*

Cite This: https://doi.org/10.1021/acsomega.2c04053

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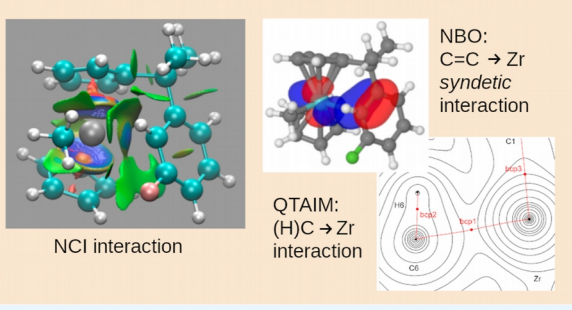
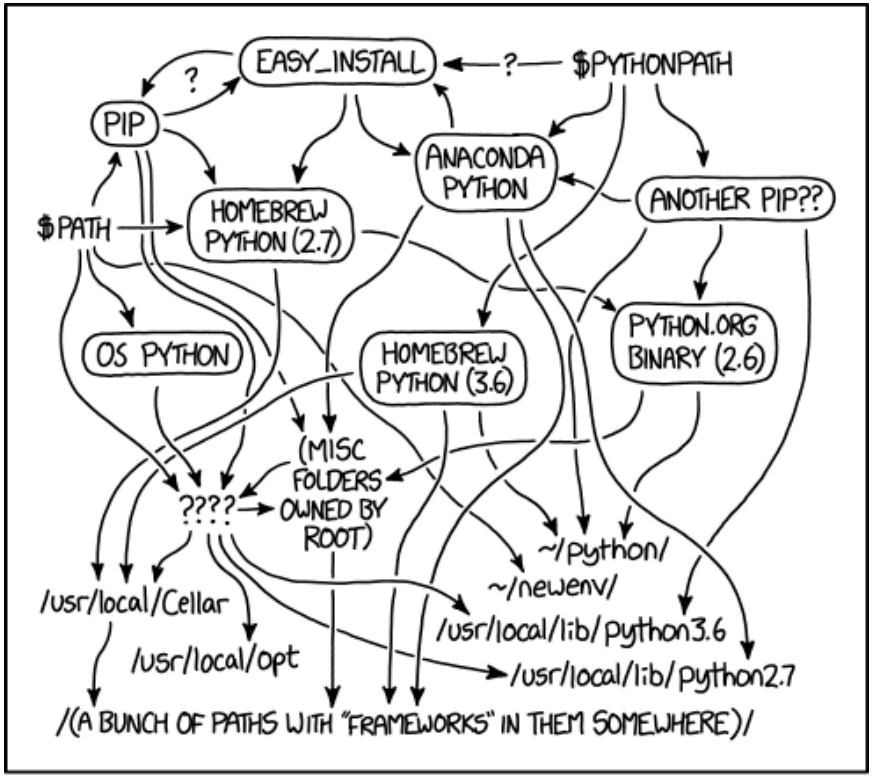
ABSTRACT: Detailed density functional theory studies at the B3LYP and PBE-D3 levels of theory were performed on the cationic compound $[Cp(C_5H_4CMe_2C_6H_4F)ZrMe]^+$, with the F atom occupying either the ortho, meta, or para positions of the arene ring. In all cases, the arene ring coordinates with the cationic zirconium metal. The nature of this coordination is such that for the meta- or para-substituted arene ring, it is predominantly the ortho carbon atom of the C−H bond which interacts with the metal, as evident from noncovalent interaction studies. This is further corroborated by the natural bond orbital and quantum theory of atoms in molecular studies. In the case of the F atom being in the ortho position, we obtained clear-cut evidence for a Zr−F coordination.



Computational Details. All calculations were performed on Debian Linux (Jessie). The B3LYP calculations were performed using Gaussian G09, version D01.[69] The PBE-D3 calculations were performed using GAMESS 2014 R1.[70,71] In all cases, a mixed basis set consisting out of Pople's 6-311G(d,p) basis set was used for all elements but Zr, where the Stuttgart−Dresden effective core basis set was used. This mixed basis set is abbreviated as ecp11 and is basically an expansion of the previously used ecp1 basis set.[28]

Installing software is easy, just follow the yellow brick road!



MY PYTHON ENVIRONMENT HAS BECOME SO DEGRADED THAT MY LAPTOP HAS BEEN DECLARED A SUPERFUND SITE.

https://xkcd.com/1987/

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Who cares how it was installed?

What does the vision look like?

There are five key qualities present in our vision of a positive science culture. Realising chemistry's potential is possible if we can collectively create a culture that is:

1. Rigorous
Science must be conducted with integrity and in a way that stands up to scrutiny. Scientists should implement good practice and follow professional standards but when there are mistakes, they should be used as opportunities for learning.

2. Safe and supportive
Avoiding causing physical, emotional and psychological harm is just one element of this cultural quality. Chemistry should be a field where scientists and innovators at all levels are provided with the required training and support they need to succeed, and where professional development is supported. Kindness and feedback should be valued, career path diversity is to be nurtured, and everyone should be open to challenge in a constructive manner.

3. Ethical and responsible
Scientists should stick to all ethical standards and consider the social benefits, moral dilemmas and potential negative impacts of their work. They should also work to enhance environmental sustainability in their workplace where possible. Meanwhile, active measures should be in place to prevent and address any bullying, discrimination and harassment so that everyone in this field feels respected.

What has the Royal Society of Chemistry committed to doing?

There are three initial priorities:

1. **Increase our efforts to share practical resources to support our community in overcoming barriers to improving the culture in the chemical sciences.**
2. **Create space for brave conversations covering areas where our community has identified tensions between the qualities of a positive science culture.**
3. **Showcase good practice examples of leadership, highlighting where leaders go above and beyond to break down barriers and open up opportunities.**

These steps are in addition to the extensive work we are already doing on inclusion and diversity, ethical practice, open science, and recognition of science and scientists.

The society will also continue to develop initiatives that support the development of a positive science culture, meaning more priorities could be added in the future.

4. Open and collaborative
Scientists should be open to questioning and the scientific community should participate in public debate to expand our collective knowledge, with data deposited in accessible formats and locations so that others can also benefit. Access to scientific publications should also be free and unrestricted where possible, and science should be conducted in a way that encourages cross-discipline and/or international collaboration where suitable.

5. Accessible and inclusive
Funders and employers should actively remove systemic constraints affecting people disadvantaged by inequalities, while individuals should take steps to reduce their conscious and implicit biases. Minoritised scientists, students and innovators should be able to feel they are part of the scientific community, supported to thrive, and accepted personally and professionally.

What happens next?

Building a positive culture where the qualities listed above are prevalent will not just benefit our community and society more generally, it will support quality science. Getting to this point, however, will require significant work over a prolonged period of time.

These qualities must be embedded through education as well as in the working world for this improved culture to last and become second nature. The statement makes it clear that it will also require support from management, leaders and organisations that have the power to facilitate progress, backing up a view raised during early consultations.

The breaking down of barriers was something that came up repeatedly during conversations and is a key part of the vision. This will require both voluntary and regulatory approaches that will also support sustainable careers and maintain high standards of professional conduct.

While the work needed – at least at the outset – to push for a more positive culture is not insignificant, the Royal Society of Chemistry is bullish in its optimism about the potential end results. Creativity, discovery and innovation would all be expected to bloom if such a culture came to be, while job satisfaction and scientific excellence are other positives awaiting science and society at large.

The five qualities apply across the three foundational blocks of a healthy scientific environment – those being scientific practice, participation, and wellbeing and development.

Foundation	Scientific practice	Participation	Wellbeing and development
What does it mean?	Scientific practice is about the way in which science is carried out. Good scientific practice is achieved when science and innovation are conducted in a rigorous, ethical and responsible way. Effective science is also open and collaborative, involving the sharing of knowledge and expertise across disciplines, sectors and countries.	Participation in science is about who is able and enabled to take part in science and innovation. Broad participation requires an inclusive and accessible environment that ensures no one is barred from contributing, and an open and collaborative approach that brings together the right knowledge and the right people to maximise the quality and impact of science and innovation.	Wellbeing is about the way people are treated, and development is about how they are empowered to achieve their potential. Workplaces that safeguard wellbeing and encourage development are inclusive and accessible, as well as safe and supportive. They also require adherence to ethical and responsible conduct to ensure that no harm is caused to anyone involved.

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Who cares how it was installed?

FEATURE

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Voice | October 2023 9

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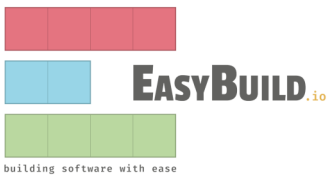
EasyBuild

- installs software and dependencies
- installs software from source
- creates module files
- 'build-files'
- more users in Europe
- open source

- prescriptive: toolchain versions (compiler version determines version of dependencies)



Spack

- installs software and dependencies
- installs software from source
- creates module files
- 'build-files'
- more users in North America
- open source

- mix & match approach (compiler version does not determine dependency version, compilation 'on the fly')

```
# J. Sassmannshausen (Imperial College London/UK)

easyblock = 'CMakeMake'

name = 'json-fortran'
version = '8.3.0'

homepage = 'https://github.com/jacobwilliams/json-fortran'
description = "JSON-Fortran: A Modern Fortran JSON API"

toolchain = {'name': 'GCCcore', 'version': '12.2.0'}

source_urls = ['https://github.com/jacobwilliams/json-fortran/archive/']
sources = ['%(version)s.tar.gz']
checksums = ['5fe9ad709a726416cec986886503e0526419742e288c4e43f63c1c22026d1e8a']

builddependencies = [
    ('binutils', '2.39'),
    ('CMake', '3.24.3'),
]

configopts = '-DUSE_GNU_INSTALL_CONVENTION=TRUE'

runtest = 'check'

sanity_check_paths = {
    'files': ['lib/libjsonfortran.a', 'lib/libjsonfortran.%s' % SHLIB_EXT],
    'dirs': ['include'],
}

moduleclass = 'lib'
```

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checksums = [
    '5fe9ad709a726416cec986886503e0526419742e288c4e43f63c1c22026d1e8a',
    '315e70c12edfe15535dbd54ac99ea66d41df3989a0917b8da7f024fdea2af609',
]

builddependencies = [
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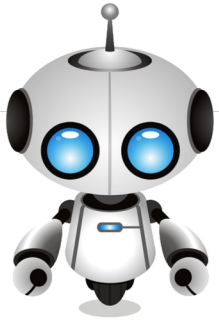
```

EasyBuild can use hooks

```
# J. Sassmannshausen (Imperial College London/UK)
def parse_hook(ec, *args, **kwargs):

    # We want to use the GROMACS wrapper from version 2023.1 onward
    if ec.name == 'GROMACS':
        if LooseVersion(ec.version) >= LooseVersion('2023.1'):
            module = 'GROMACS-plugin'
            module_version = '2.0.3' # Version of plugin
            dep_type = 'dependencies'

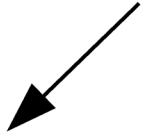
    if dep_type:
        add_extra_dependencies(ec, dep_type, module, module_version)
```



(c) https://pixabay.com/

Introduction to EasyBob

```
GROMACS-2023.1-foss-2022a-CUDA-11.7.0.eb
```



```
./automated-install.sh /full/path/to/softwarelist.txt
```

EasyBob creates submission scripts for our PBSPro queue and submits them to the cluster. Due to our heterogeneous environment (Intel, AMD), we are building software micro-architecture specific to gain the best performance from the build. As it is automated, software within EasyBuild can be installed automatically within say 1 day.

We are planning to release the set of scripts soon, so watch this space!

European **E**nvironment for **S**cientific **S**oftware **I**nstallation (EESSI)

European **E**nvironment for **S**cientific **S**oftware **I**nstallation (EESSI)

Instead of installing software again and again on various HPC clusters, both locally and at other sites, we only do the building once but for different architecture (AMD, Intel, ARM) and different micro-architectures (Icelake, Skylake, Zen3, Zen4, aarch64…) as well as GPUs (NVIDIA, AMD, Intel). Distributing the so created binaries using CernVM-FS, using an initialisation script to ‘mount’ the correct binary for a given CPU results in a sustainable way of software installation.

Due to the use of CernVM-FS, and OS abstraction layer and a few other ‘tricks’ it is possible to run the **same** software stack on for example the HPC cluster, a MacOS laptop, and a Windows desktop. This is ideal for researcher to test out input files (pre-processing of data) or do some more more interactive post-processing of a large calculation

Further readings

EasyBuild:
https://easybuild.io/

TechTalks:
https://easybuild.io/tech-talks/

Tutorials:
https://tutorial.easybuild.io/2023-eb-eessi-uk-workshop/

EESSI:
https://eessi.io/
https://www.multixscale.eu/

Spack:
https://spack.io/