Automating data sharing through authoring tools - Supporting information

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1 Introduction

This supporting information provides additional context on the extent of use of org-mode in publishing, as well as some screenshots on what org-mode looks like and how it renders into PDF and HTML.

Supporting information: 

2 Other published papers that used org-mode

One of the authors (Kitchin) has used org-mode extensively in scientific publishing in over a dozen peer-reviewed papers.

1. Alexander P. Hallenbeck and John R. Kitchin. Effects of O_2 and SO_2 on the capture capacity of a primary-amine based polymeric CO_2 sorbent. *Industrial & Engineering Chemistry Research*, 52(31):10788–10794, 2013

2. Spencer D. Miller, Vladimir V. Pushkarev, Andrew J. Gellman, and John R. Kitchin. Simulating temperature programmed desorption of oxygen on Pt(111) using DFT derived coverage dependent desorption barriers. *Topics in Catalysis*, 57(1-4):106–117, 2014

3. Zhongnan Xu and John R. Kitchin. Probing the coverage dependence of site and adsorbate configurational correlations on (111) surfaces of late transition metals. *J. Phys. Chem. C*, 118(44):25597–25602, 2014

4. Zhongnan Xu and John R. Kitchin. Relating the electronic structure and reactivity of the 3d transition metal monoxide surfaces. *Catalysis Communications*, 52:60–64, 2014

5. Matthew T. Curnan and John R. Kitchin. Effects of concentration, crystal structure, magnetism, and electronic structure method on first-principles oxygen vacancy formation energy trends in perovskites. *The Journal of Physical Chemistry C*, 118(49):28776–28790, 2014

6. John R. Kitchin. Data sharing in surface science. *Surface Science*, N/A:in press, 2015

7. John R. Kitchin. Examples of effective data sharing in scientific publishing. *ACS Catalysis*, 5(6):3894–3899, 2015

8. Prateek Mehta, Paul A. Salvador, and John R. Kitchin. Identifying potential BO_2 oxide polymorphs for epitaxial growth candidates. *ACS Appl. Mater. Interfaces*, 6(5):3630–3639, 2015

9. Zhongnan Xu, Jan Rossmeisl, and John R. Kitchin. A linear response DFT+U study of trends in the oxygen evolution activity of transition metal rutile dioxides. *The Journal of Physical Chemistry C*, 119(9):4827–4833, 2015

10. Zhongnan Xu and John R. Kitchin. Relationships between the surface electronic and chemical properties of doped 4d and 5d late transition metal dioxides. *The Journal of Chemical Physics*, 142(10):104703, 2015

11. Zhongnan Xu and John R Kitchin. Tuning oxide activity through modification of the crystal and electronic structure: From strain to potential polymorphs. *Phys. Chem. Chem. Phys.*, 17:28943–28949, 2015

12. Jacob R. Boes, Gamze Gumuslu, James B. Miller, Andrew J. Gellman, and John R. Kitchin. Estimating bulk-composition-dependent H_2 adsorption energies on Cu_xPd_{1-x} alloy (111) surfaces. *ACS Catalysis*, 5:1020–1026, 2015

13. Jacob R. Boes, Mitchell C. Groenenboom, John A. Keith, and John R. Kitchin. Neural network and reaxff comparison for Au properties. *Accepted 1/2016, Int. J. Quantum Chemistry*, 2016

Many of these papers include extensive supporting information files that include the org-mode source of the manuscript, as well as data files used in the papers.

There are other examples of org-mode in the literature as well [14–16].

3 Tables

This section shows an example of an org-mode table in Fig. 1 on the left, and how it is rendered in the PDF. The data in the table is automatically extracted and saved as a comma-separated value file that is attached to the PDF. The HTML version is shown in Fig.2.

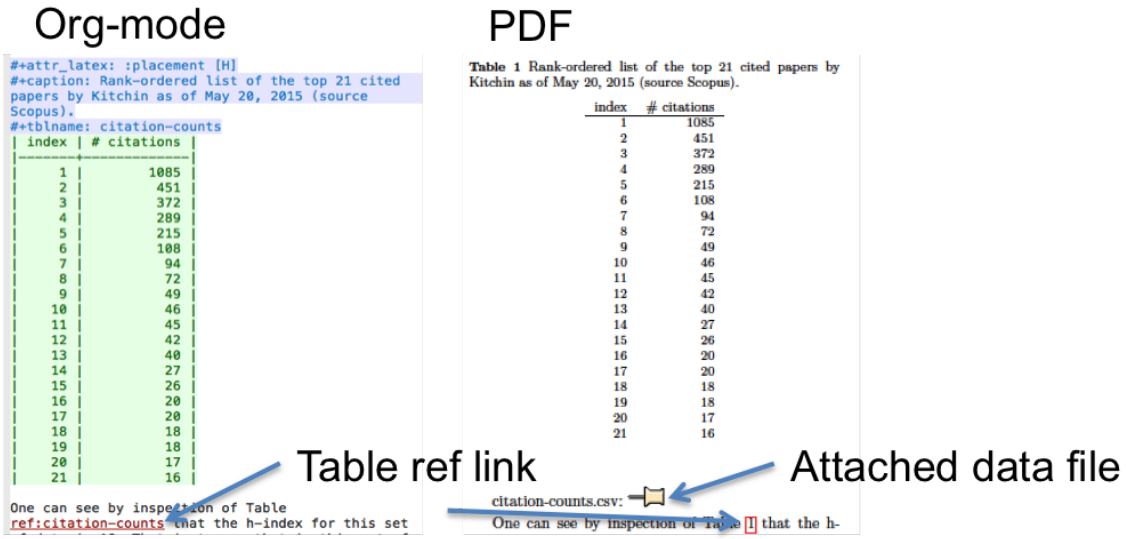


Figure 1: Comparison of the org-mode table and table rendered in the PDF file.

Figure 2: The HTML rendered table and corresponding generated HTML code. .

4 Code

Fig. 3 shows an example of a code block in org-mode and the rendered code on the right. The code is automatically extracted in the conversion and embedded in the pdf. The corresponding export to HTML is shown in Fig. 4 along with the generated HTML for this code block.

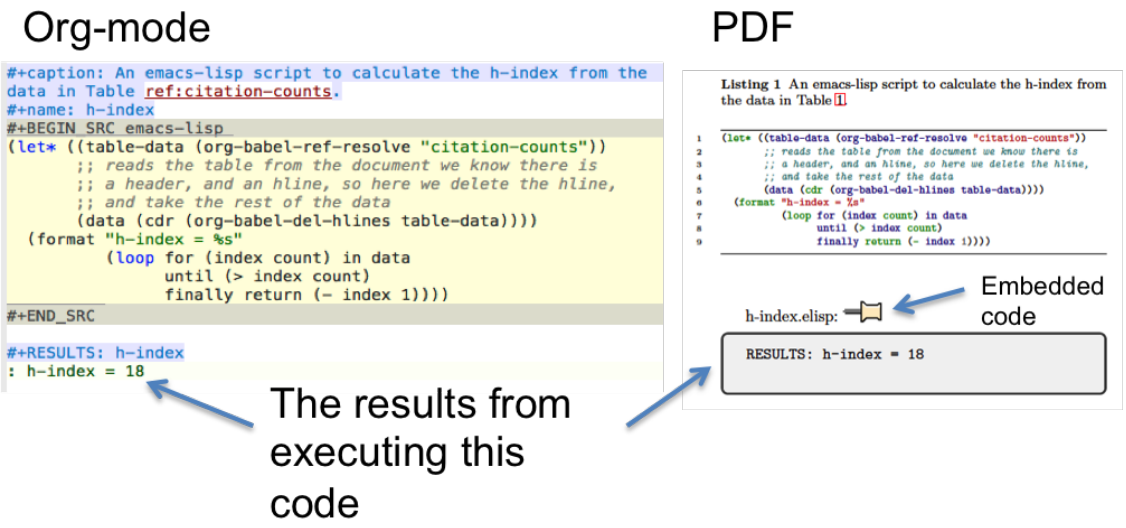
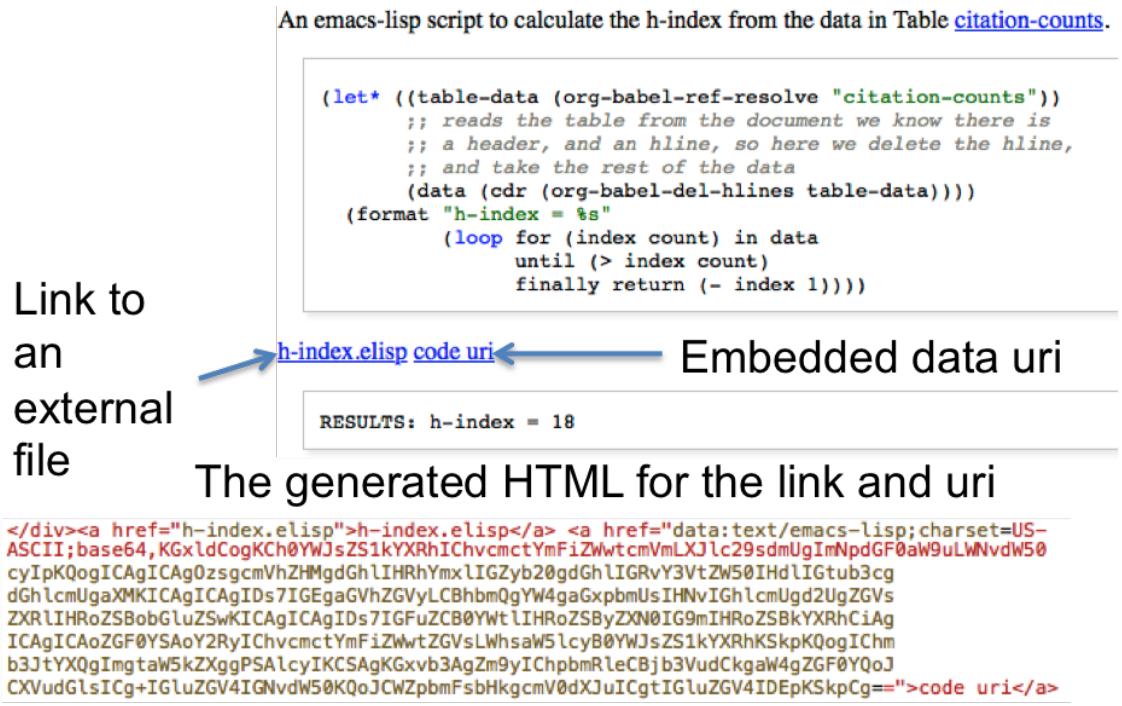


Figure 3: Comparison of code in org-mode (left), and rendered in the PDF file (right).




```
</div><a href="h-index.elisp">h-index.elisp</a> <a href="data:text/emacs-lisp;charset=US-
ASCII;base64,KGxldCogKCh0YWJsZS1kYXRhIChvcmctYmFiZWwtcmVmLXJlc29sdmUgImNpdGF0aW9uLWNvdW50
cyIpKQogICAgICAgOzsgcmVhZHMgdGhlIHRhYmxlIGZyb20gdGhlIGRvY3VtZW50IHdlIGtub3cg
dGhlcmUgaXMKICAgICAgIDs7IGEgaGVhZGVyLCBhbmQgYW4gaxpbmUsIHNvIGhlcmUgd2UgZGVs
ZXRlIHRoZSBobGluZSwKICAgICAgIDs7IGFuZCB0YWtlIHRoZSByZXN0IG9mIHRoZSBkYXRhCiAg
ICAgICAoZGF0YSAoY2RyIChvcmctYmFiZWwtZGVsLWhsaW5lcyB0YWJsZS1kYXRhKSkpQogICAg
b3JtYXQgImgtaW5kZXggPSAlcyIKCSAgKGxvb3AgZm9yIChpbmRleCBjb3VudCkgaW4gZGF0YQoJ
CXVudGlsICg+IGluZGV4IGNvdW50KQoJCWZpbmFsbHkgcmV0dXJuICgtIGluZGV4IDEpKSkpCg==">code uri</a>
```

Figure 4: The HTML rendered table and the generated code.

5 PDF attachments

Figure 5 shows what a PDF file with attachments in it looks like in Adobe Acrobat Pro. Not all PDF readers support attachments.

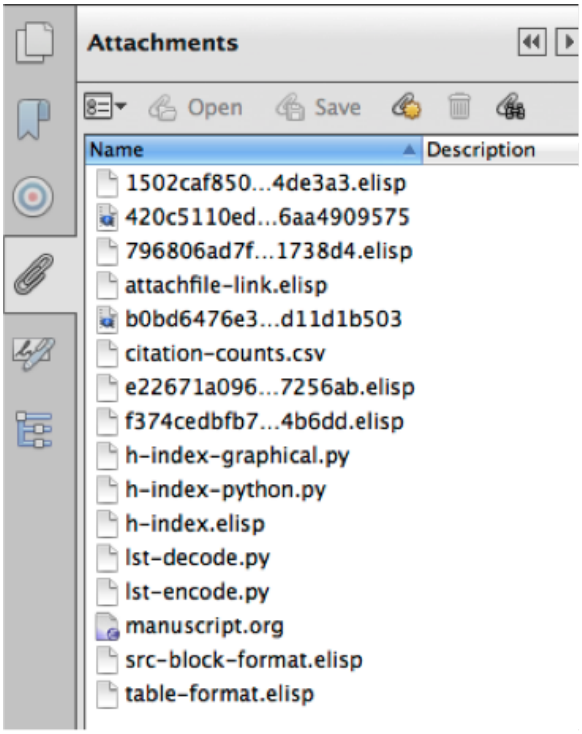


Figure 5: Screenshot of PDF attachments in Adobe Acrobat.

References

[1] Alexander P. Hallenbeck and John R. Kitchin. Effects of O_2 and SO_2 on the capture capacity of a primary-amine based polymeric CO_2 sorbent. *Industrial & Engineering Chemistry Research*, 52(31):10788–10794, 2013.

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[12] Jacob R. Boes, Gamze Gumuslu, James B. Miller, Andrew J. Gellman, and John R. Kitchin. Estimating bulk-composition-dependent H_2 adsorption energies on Cu_xPd_{1-x} alloy (111) surfaces. *ACS Catalysis*, 5:1020–1026, 2015.

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