# cs109a\_hw1

September 19, 2018

# 1 CS109A Introduction to Data Science

# 1.1 Homework 1: Data Collection - Web Scraping - Data Parsing

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```
In [2]: ## RUN THIS CELL TO GET THE RIGHT FORMATTING
     import requests
     from IPython.core.display import HTML
     styles = requests.get("https://raw.githubusercontent.com/Harvard-IACS/2018-CS109A/mast-HTML(styles)
```

Out[2]: <IPython.core.display.HTML object>

## **Instructions**

- To submit your assignment follow the instructions given in Canvas.
- The deliverables in Canvas are:
  - a) This python notebook with your code and answers, plus a pdf version of it (see Canvas for details),
  - b) the bibtex file you created,
  - c) The CSV file you created,
  - d) The JSON file you created.
- Exercise **responsible scraping**. Web servers can become slow or unresponsive if they receive too many requests from the same source in a short amount of time. Use a delay of 10 seconds between requests in your code. This helps not to get blocked by the target website. Run the webpage fetching part of the homework only once and do not re-run after you have saved the results in the JSON file (details below).
- Web scraping requests can take several minutes. This is another reason why you should not
  wait until the last minute to do this homework.
- For this assignment, we will use Python 3.5 for grading.

# 2 Data Collection - Web Scraping - Data Parsing

In this homework, your goal is to learn how to acquire, parse, clean, and analyze data. Initially you will read the data from a file, and then later scrape them directly from a website. You will look

for specific pieces of information by parsing the data, clean the data to prepare them for analysis, and finally, answer some questions.

In doing so you will get more familiar with three of the common file formats for storing and transferring data, which are: - CSV, a text-based file format used for storing tabular data that are separated by some delimiter, usually comma or space. - HTML/XML, the stuff the web is made of. - JavaScript Object Notation (JSON), a text-based open standard designed for transmitting structured data over the web.

# 2.1 Help a professor parse their publications and extract information.

#### 2.1.1 Overview

In this part your goal is to parse the HTML page of a professor containing some of his/her publications, and answer some questions. This page is provided to you in the file data/publist\_super\_clean.html. There are 45 publications in descending order from No. 244 to No. 200.

Question 1 [40 pts]: Parsing and Converting to bibTex and CSV using Beautiful Soup and python string manipulation

A lot of the bibliographic and publication information is displayed in various websites in a not-so-structured HTML files. Some publishers prefer to store and transmit this information in a .bibTex file which looks roughly like this (we've simplified a few things):

```
@article {
    author = "John Doyle"
    title = "Interaction between atoms"
    URL = "Papers/PhysRevB_81_085406_2010.pdf"
    journal = "Phys. Rev. B"
    volume = "81"
}
```

You will notice that this file format is a set of items, each of which is a set of key-value pairs. In the python world, you can think of this as a list of dictionaries. If you think about spreadsheets

(as represented by CSV files), they have the same structure. Each line is an item, and has multiple features, or keys, as represented by that line's value for the column corresponding to the key.

You are given an .html file containing a list of papers scraped from the author's website and you are to write the information into .bibTex and .CSV formats. A useful tool for parsing websites is BeautifulSoup (http://www.crummy.com/software/BeautifulSoup/) (BS). In this problem, will parse the file using BS, which makes parsing HTML a lot easier.

- **1.1** Write a function called make\_soup that accepts a filename for an HTML file and returns a BS object.
- **1.2** Write a function that reads in the BS object, parses it, converts it into a list of dictionaries: one dictionary per paper. Each of these dictionaries should have the following format (with different values for each publication):

```
{'author': 'L.A. Agapito, N. Kioussis and E. Kaxiras',
  'title': '"Electric-field control of magnetism in graphene quantum dots:\n Ab initio calculat
  'URL': 'Papers/PhysRevB_82_201411_2010.pdf',
  'journal': 'Phys. Rev. B',
  'volume': '82'}
```

- **1.3** Convert the list of dictionaries into standard .bibTex format using python string manipulation, and write the results into a file called publist.bib.
- **1.4** Convert the list of dictionaries into standard tabular .csv format using pandas, and write the results into a file called publist.csv. The csv file should have a header and no integer index.

## **HINT**

- Inspect the HTML code for tags that indicate information chunks such as title of the paper. The find\_all method of BeautifulSoup might be useful.
- Question 1.2 is better handled if you break the code into functions, each performing a small task such as finding the author(s) for each paper.
- Question 1.3 is effectively tackled by first using python string formatting on a template string.
- Make sure you catch exceptions when needed.
- Make sure you check for **missing data** and handle these cases as you see fit.

### Resources

- BeautifulSoup Tutorial.
- More about the BibTex format.

#### 2.1.2 Answers

1.1 Write a function called make\_soup ...

```
Arqs:
                   filename: A string name of the file.
               Returns:
                   A BS object containing the HTML page ready to be parsed.
            # your code here
            with open(filename, 'r') as f:
                html_text = f.read()
            return BeautifulSoup(html_text, 'html.parser')
In [13]: # check your code - print the BS object, you should get a familiar HTML page as text
         # clear/remove output before making pdf
         #soup = make_soup(PUB_FILENAME)
         #print(soup)
  Your output should look like this:
<!DOCTYPE HTML PUBLIC "-//W3C//DTD HTML 4.01 Transitional//EN"</pre>
   "http://www.w3.org/TR/html4/loose.dtd">
<title>Kaxiras E journal publications</title>
<head>
<meta content="text/html;charset=utf-8" http-equiv="Content-Type"/>
<link href="../styles/style pubs.css" rel="stylesheet" type="text/css"/>
<meta content="" name="description"/>
<meta content="Kaxiras E, Multiscale Methods, Computational Materials" name="keywords"/>
</head>
<body>

    start="244">

<1i>>
<a href="Papers/2011/PhysRevB 84_125411_2011.pdf" target="paper244">
"Approaching the intrinsic band gap in suspended high-mobility graphene nanoribbons"</a>
<br/>Sming-Wei Lin, Cheng Ling, Luis A. Agapito, Nicholas Kioussis, Yiyang Zhang, Mark Ming-Cheng
<i>PHYSICAL REVIEW B </i> <b>84</b>, 125411 (2011)
<br/>
<
<a href="Papers/2011/PhysRevB_84_035325_2011.pdf" target="paper243">
"Effect of symmetry breaking on the optical absorption of semiconductor nanoparticles"</a>
<br/>br/>JAdam Gali, Efthimios Kaxiras, Gergely T. Zimanyi, Sheng Meng,
<i>PHYSICAL REVIEW B </i> <b>84</b>, 035325 (2011)
\langle br/ \rangle
```

. . .

1.2 Write a function that reads in the BS object, parses it, converts it into a list of dictionaries...

```
In [8]: # clear output before making pdf
        # your code here
        def list_of_html_citations(soup):
            body = soup.find('body')
            return body.find_all('ol')
        def clean_text(text):
            text_to_strip = ['\n',' ',',']
            for t in text_to_strip:
                text = text.strip(t)
            text = text.replace("\n"," ")
            return text
        def get_title(citation):
            text = citation.find('a').get_text()
            return clean_text(text)
        def get_author(citation):
            text = citation.find('li').contents[4]
            return clean_text(text)
        def get_url(citation):
            text = citation.find('a').get('href')
            return clean_text(text)
        def get_journal(citation):
            text = citation.find('i').get_text()
            return clean_text(text)
        def get_volume(citation):
            tag = citation.find('b')
            if tag is None:
                return None
            else:
                text = tag.get_text()
                return clean_text(text)
        def create_citation_dict(citation):
            return {
                'author': get_author(citation),
                'title': get_title(citation),
                'URL': get_url(citation),
```

```
'volume': get_volume(citation)
            }
        def parse_for_citations(soup):
            return [create_citation_dict(c) for c in list_of_html_citations(soup)]
In [9]: # your code here
       parse_for_citations(soup)
Out[9]: [{'author': 'Ming-Wei Lin, Cheng Ling, Luis A. Agapito, Nicholas Kioussis, Yiyang Zhan
          'title': '"Approaching the intrinsic band gap in suspended high-mobility graphene na
          'URL': 'Papers/2011/PhysRevB_84_125411_2011.pdf',
          'journal': 'PHYSICAL REVIEW B',
          'volume': '84'},
         {'author': 'JAdam Gali, Efthimios Kaxiras, Gergely T. Zimanyi, Sheng Meng',
          'title': '"Effect of symmetry breaking on the optical absorption of semiconductor na
          'URL': 'Papers/2011/PhysRevB_84_035325_2011.pdf',
          'journal': 'PHYSICAL REVIEW B',
          'volume': '84'},
         {'author': 'Jan M. Knaup, Han Li, Joost J. Vlassak, and Efthimios Kaxiras',
          'title': '"Influence of CH2 content and network defects on the elastic properties of
          'URL': 'Papers/2011/PhysRevB_83_054204_2011.pdf',
          'journal': 'PHYSICAL REVIEW B',
          'volume': '83'},
         {'author': 'Martin Heiss, Sonia Conesa-Boj, Jun Ren, Hsiang-Han Tseng, Adam Gali',
          'title': '"Direct correlation of crystal structure and optical properties in wurtzit
          'URL': 'Papers/2011/PhysRevB_83_045303_2011.pdf',
          'journal': 'PHYSICAL REVIEW B',
          'volume': '83'},
         {'author': 'Simone Melchionna, Efthimios Kaxiras, Massimo Bernaschi and Sauro Succi',
          'title': '"Endothelial shear stress from large-scale blood flow simulations"',
          'URL': 'Papers/2011/PhilTransRSocA_369_2354_2011.pdf',
          'journal': 'Phil. Trans. R. Soc. A',
          'volume': '369'},
         {'author': 'J R Maze, A Gali, E Togan, Y Chu, A Trifonov',
          'title': '"Properties of nitrogen-vacancy centers in diamond: the group theoretic ap
          'URL': 'Papers/2011/NewJPhys_13_025025_2011.pdf',
          'journal': 'New Journal of Physics',
          'volume': '13'},
         {'author': 'Kejie Zhao, Wei L. Wang, John Gregoire, Matt Pharr, Zhigang Suo',
          'title': '"Lithium-Assisted Plastic Deformation of Silicon Electrodes in Lithium-Ion
          'URL': 'Papers/2011/NanoLett_11_2962-2967_2011.pdf',
          'journal': 'Nano Lett.',
          'volume': '11'},
         {'author': 'Masataka Katono, Takeru Bessho, Sheng Meng, Robin Humphry-Baker, Guido Ro
          'title': '"D--A Dye System Containing Cyano-Benzoic Acid as Anchoring Group for Dye-
```

'journal': get\_journal(citation),

```
'URL': 'Papers/2011/Langmuir_27_14248_2011.pdf',
 'journal': 'Langmuir',
 'volume': '27'},
{'author': 'Thomas D. Kuhne, Tod A. Pascal, Efthimios Kaxiras, and Yousung Jung',
 'title': '"New Insights into the Structure of the Vapor/Water Interface from Large-S
 'URL': 'Papers/2011/JPhysChemLett_2_105-113_2011.pdf',
 'journal': 'J. Phys. Chem. Lett.',
 'volume': '2'},
{'author': 'Sheng Meng, Efthimios Kaxiras, Md. K. Nazeeruddin, and Michael Gratzel',
 'title': '"Design of Dye Acceptors for Photovoltaics from First-Principles Calculati
 'URL': 'Papers/2011/JPhysChemC_115_9276-9282_2011.pdf',
 'journal': 'J. Phys. Chem. C',
 'volume': '115'},
{'author': 'Bingjun Xu, Jan Haubrich, Thomas A. Baker, Efthimios Kaxiras, and Cynthia
 'title': '"Theoretical Study of O-Assisted Selective Coupling of Methanol on Au(111)
 'URL': 'Papers/2011/JPhysChemC_115_3703-3708_2011.pdf',
 'journal': 'J. Phys. Chem. C',
 'volume': '115'},
{'author': 'Jun Ren, Sheng Meng, Yi-Lin Wang, Xu-Cun Ma, Qi-Kun Xue, Efthimios Kaxira
 'title': '"Properties of copper (fluoro-)phthalocyanine layers deposited on epitaxia
 'URL': 'Papers/2011/JChemPhys_134_194706_2011.pdf',
 'journal': 'J. Chem. Phys.',
 'volume': '134'},
{'author': 'Jan Haubrich, Efthimios Kaxiras, and Cynthia M. Friend',
 'title': '"The Role of Surface and Subsurface Point Defects for Chemical Model Studi
 'URL': 'Papers/2011/Chemistry_17_4496-4506_2011.pdf',
 'journal': 'Chem. Eur. J.',
 'volume': '17'},
{'author': 'Thomas A. Baker, Bingjun Xu, Stephen C. Jensen, Cynthia M. Friend and Eft.
 'title': '"Role of defects in propene adsorption and reaction on a partially O-cover
 'URL': 'Papers/2011/CatalSciTechnol_1_1166_2011.pdf',
 'journal': 'Catal. Sci. Technol.',
 'volume': '1'},
{'author': 'Youdong Mao, Wei L. Wang, Dongguang Wei, Efthimios Kaxiras, and Joseph G.
 'title': '"Graphene Structures at an Extreme Degree of Buckling"',
 'URL': 'Papers/2011/ACSNano_5_1395-1400_2011.pdf',
 'journal': 'ACSNano.',
 'volume': '5'},
{'author': 'H. Li, J.M. Knaup, E. Kaxiras and J.J. Vlassak',
 'title': '"Stiffening of organosilicate glasses by organic cross-linking"',
 'URL': 'Papers/ActaMater_59_44-52_2011.pdf',
 'journal': 'Acta Mater.',
 'volume': '59'},
{'author': 'W.L. Wang and E. Kaxiras',
 'title': '"Graphene hydrate: theoretical prediction of a new insulating form of gray
 'URL': 'Papers/NewJPhys_12_125012_2010.pdf',
 'journal': 'New J. Phys.',
 'volume': '12'},
```

```
{'author': 'L.A. Agapito, N. Kioussis and E. Kaxiras',
 'title': '"Electric-field control of magnetism in graphene quantum dots: Ab initio
 'URL': 'Papers/PhysRevB_82_201411_2010.pdf',
 'journal': 'Phys. Rev. B',
 'volume': '82'},
{'author': 'A. Peters, S. Melchionna, E. Kaxiras, J. Latt, J. Sircar, S. Succi',
 'title': '"Multiscale simulation of cardiovascular flows on the IBM Bluegene/P:
 'URL': 'Papers/IEEE-SC10_2010.pdf',
 'journal': '2010 ACM/IEEE International Conference for High Performance',
 'volume': None},
{'author': 'J. Ren, E. Kaxiras and S. Meng',
 'title': '"Optical properties of clusters and molecules from real-time time-dependent
 'URL': 'Papers/MolPhys_108_1829-1844_2010.pdf',
 'journal': 'Molec. Phys.',
 'volume': '108'},
{'author': 'T.A. Baker, E. Kaxiras and C.M. Friend',
 'title': '"Insights from Theory on the Relationship Between Surface Reactivity and G
 'URL': 'Papers/TopicsCatal_53_365-377_2010.pdf',
 'journal': 'Top. Catal.',
 'volume': '53'},
{'author': 'H.P. Chen, R.K. Kalia, E. Kaxiras, G. Lu, A. Nakano, K. Nomura',
 'title': '"Embrittlement of Metal by Solute Segregation-Induced Amorphization"',
 'URL': 'Papers/PhysRevLett_104_155502_2010.pdf',
 'journal': 'Phys. Rev. Lett.',
 'volume': '104'},
{'author': 'S. Meng and E. Kaxiras',
 'title': '"Electron and Hole Dynamics in Dye-Sensitized Solar Cells: Influencing Fac
 'URL': 'Papers/NanoLett_10_1238-1247_2010.pdf',
 'journal': 'NanoLett.',
 'volume': '10'},
{'author': 'C.L. Chang, S.K.R.S. Sankaranarayanan, D. Ruzmetov, M.H. Engelhard, E. Ka
 'title': '"Compositional tuning of ultrathin surface oxides on metal and alloy subst:
 'URL': 'Papers/PhysRevB_81_085406_2010.pdf',
 'journal': 'Phys. Rev. B',
 'volume': '81'},
{'author': 'T.A. Baker, C.M. Friend and E. Kaxiras',
 'title': '"Local Bonding Effects in the Oxidation of CO on Oxygen-Covered Au(111) fr
 'URL': 'Papers/JChemTheComp_6_279-287_2010.pdf',
 'journal': 'J. Chem. Theory Comput.',
 'volume': '6'},
{'author': 'S. Melchionna, M. Bernaschi, S. Succi, E. Kaxiras, F.J. Rybicki, D. Mitso
 'title': '"Hydrokinetic approach to large-scale cardiovascular blood flow"',
 'URL': 'Papers/CompPhysComm_181_462-472_2010.pdf',
 'journal': 'Comp. Phys. Comm.',
 'volume': '181'},
{'author': 'M. Bernaschi, M. Fatica, S. Melchionna, S. Succi and E. Kaxiras',
 'title': '"A flexible high-performance Lattice Boltzmann GPU code for the simulation
 'URL': 'Papers/ConcComp_22_1-14_2010.pdf',
```

```
'journal': 'Concurrency Computat.: Pract. Exper.',
 'volume': '22'},
{'author': 'E. Manousakis, J. Ren, S. Meng and E. Kaxiras',
 'title': '"Is the nature of magnetic order in copper-oxides and iron-pnictides diffe
 'URL': 'Papers/SolStComm_150_62-65_2010.pdf',
 'journal': 'Sol. St. Comm.',
 'volume': '150'},
{'author': 'A. Gali, E. Janzen, P. Deak, G. Kresse and E. Kaxiras',
 'title': '"Theory of Spin-Conserving Excitation of the N-V Center in Diamond"',
 'URL': 'Papers/PhysRevLett_103_186404_2009.pdf',
 'journal': 'Phys. Rev. Lett.',
 'volume': '103'},
{'author': 'S.K.R.S. Sankaranarayanan, E. Kaxiras and S. Ramanathan',
 'title': '"Electric field tuning of oxygen stoichiometry at oxide surfaces: molecula:
 'URL': 'Papers/EnEnviSci_2_1196-1204_2009.pdf',
 'journal': 'Energy & Environmental Sci.',
 'volume': '2'},
{'author': 'M. Bernaschi, S. Melchionna, S. Succi, M. Fyta, E. Kaxiras',
 'title': '"MUPHY: A parallel MUlti PHYsics/scale code for high performance bio-flui
 'URL': 'Papers/CompPhysComm_180_1495-1502_2009.pdf',
 'journal': 'Comp. Phys. Comm.',
 'volume': '180'},
{'author': 'T.A. Baker, B.J. Xu, X.Y. Liu, E. Kaxiras and C.M. Friend',
 'title': '"Nature of Oxidation of the Au(111) Surface: Experiment and Theoretical In
 'URL': 'Papers/JPhysChemC_113_16561-16564_2009.pdf',
 'journal': 'J. Phys. Chem. C',
 'volume': '113'},
{'author': 'F.J. Rybicki, S. Melchionna, D. Mitsouras, A.U. Coskun, A.G. Whitmore, E.
 'title': '"Prediction of coronary artery plaque progression and potential rupture fr
 'URL': 'Papers/IntJCardImag_25_289-299_2009.pdf',
 'journal': 'Int. J. Cardiovasc. Imaging',
 'volume': '25'},
{'author': 'H. Chen, W.G. Zhu, E. Kaxiras, and Z.Y. Zhang',
 'title': '"Optimization of Mn doping in group-IV-based dilute magnetic semiconductors
 'URL': 'Papers/PhysRevB_79_235202_2009.pdf',
 'journal': 'Phys. Rev. B',
 'volume': '79'},
{'author': 'M. Fyta, S. Melchionna, M. Bernaschi, E. Kaxiras and S. Succi',
 'title': '"Numerical simulation of conformational variability in biopolymer transloc
 'URL': 'Papers/JStatMech_2009.pdf',
 'journal': 'J. Stat. Mech: Th. and Exper.',
 'volume': '06'},
{'author': 'E.M. Kotsalis, J.H. Walther, E. Kaxiras and P. Koumoutsakos',
 'title': '"Control algorithm for multiscale flow simulations of water"',
 'URL': 'Papers/PhysRevE_79_045701RC_2009.pdf',
 'journal': 'Phys. Rev. E - Rap. Comm.',
 'volume': '79'},
{'author': 'C.E. Lekka, J. Ren, S. Meng and E. Kaxiras',
```

```
'title': '"Structural, Electronic, and Optical Properties of Representative Cu-Flavo:
 'URL': 'Papers/JPhysChemB_113_6478_2009.pdf',
 'journal': 'J. Phys. Chem. B',
 'volume': '113'},
{'author': 'W.L. Wang, O.V. Yazyev, S. Meng and E. Kaxiras',
 'title': '"Topological Frustration in Graphene Nanoflakes: Magnetic Order and Spin L
 'URL': 'Papers/PhysRevLett_102_157201_2009.pdf',
 'journal': 'Phys. Rev. Lett.',
 'volume': '102'},
{'author': 'A. Gali and E. Kaxiras',
 'title': '"Comment on \'Ab initio Electronic and Optical Properties of the N-V-Cente
 'URL': 'Papers/PhysRevLett_102_149703_2009.pdf',
 'journal': 'Ab initio',
 'volume': '102'},
{'author': 'S. Melchionna, M. Bernaschi, M. Fyta, E. Kaxiras and S. Succi',
 'title': '"Quantized biopolymer translocation through nanopores: Departure from simp
 'URL': 'Papers/PhysRevE_79_030901RC_2009.pdf',
 'journal': 'Phys. Rev. E - Rap. Comm.',
 'volume': '79'},
{'author': 'S.K.R.S. Sankaranarayanan, E. Kaxiras, S. Ramanathan',
 'title': '"Atomistic Simulation of Field Enhanced Oxidation of Al(1000) Beyond the M
 'URL': 'Papers/PhysRevLett_102_095504_2009.pdf',
 'journal': 'Phys. Rev. Lett.',
 'volume': '102'},
{'author': 'T.A. Baker, C.M. Friend and E. Kaxiras',
 'title': '"Effects of chlorine and oxygen coverage on the structure of the Au(111) s
 'URL': 'Papers/JChemPhys_130_084701_2009.pdf',
 'journal': 'J. Chem. Phys.',
 'volume': '130'},
{'author': 'T.A. Baker, C.M. Friend and E. Kaxiras',
 'title': '"Atomic Oxygen Adsorption on Au(111) Surfaces with Defects"',
 'URL': 'Papers/JPhysChemC_113_3232_2009.pdf',
 'journal': 'J. Phys. Chem. C',
 'volume': '113'},
{'author': 'E. Kaxiras and S. Succi',
 'title': '"Multiscale simulations of complex systems: computation meets reality"',
 'URL': 'Papers/SciModSim_15_59_2008.pdf',
 'journal': 'Sci. Model. Simul.',
 'volume': '15'},
{'author': 'E. Manousakis, J. Ren, S. Meng and E. Kaxiras',
 'title': '"Effective Hamiltonian for FeAs-based superconductors"',
 'URL': 'Papers/PhysRevB_78_205112_2008.pdf',
 'journal': 'Phys. Rev. B',
 'volume': '78'}]
```

1.3 Convert the list of dictionaries into the .bibTex format using python string manipulation (python string formatting on a template string is particularly useful)..

```
In [10]: # your code here
```

```
def create_bibtex(citation_list):
             with open("publist.bib", "w") as f:
                 for c in citation_list:
                     if c['volume'] is None:
                          f.write('@article{\n\tauthor = "%s"\n\ttitle = %s\n\tURL = "%s"\n\tjo
                              % (c['author'],c['title'],c['URL'],c['journal']))
                     else:
                          f.write('@article{\n\tauthor = "%s"\n\ttitle = %s\n\tURL = "%s"\n\tjo
                              % (c['author'],c['title'],c['URL'],c['journal'],c['volume']))
In [11]: # your code here
         citation_list = parse_for_citations(soup)
         create_bibtex(citation_list)
In [14]: # check your answer - print the bibTex file
         # clear/remove output before making pdf
         #f = open('publist.bib', 'r')
         #print (f.read())
   Your output should look like this
@article{
     author = "Ming-Wei Lin, Cheng Ling, Luis A. Agapito, Nicholas Kioussis, Yiyang Zhang, Mar
     title = "Approaching the intrinsic band gap in suspended high-mobility graphene nanoribbo
     URL = "Papers/2011/PhysRevB_84_125411_2011.pdf",
     journal = "PHYSICAL REVIEW B",
     volume = 84
}
@article{
     author = "E. Kaxiras and S. Succi",
     title = "Multiscale simulations of complex systems: computation meets reality",
     URL = "Papers/SciModSim_15_59_2008.pdf",
     journal = "Sci. Model. Simul.",
     volume = 15
}
   ** 1.4 Convert the list of dictionaries into the .csv format using pandas, and write the data into
publist.csv. The csv file should have a header and no integer index...**
In [457]: # make sure you use head() when printing the dataframe
          # your code here
          def convert_to_pandas(citation_list):
              return pd.DataFrame(citation_list)
```

```
citations_pd.head()
Out [457]:
                                                       URL
                  Papers/2011/PhysRevB_84_125411_2011.pdf
                                                            Ming-Wei Lin, Cheng Ling, Luis A. A
          1
                  Papers/2011/PhysRevB_84_035325_2011.pdf
                                                            JAdam Gali, Efthimios Kaxiras, Gerg
          2
                  Papers/2011/PhysRevB_83_054204_2011.pdf
                                                            Jan M. Knaup, Han Li, Joost J. Vlas
                  Papers/2011/PhysRevB_83_045303_2011.pdf
                                                            Martin Heiss, Sonia Conesa-Boj, Jun
          3
             Papers/2011/PhilTransRSocA_369_2354_2011.pdf
                                                            Simone Melchionna, Efthimios Kaxira
In [458]: # your code here
          citations_pd.to_csv("publist.csv", index = False)
In [459]: !head -3 publist.csv
URL, author, journal, title, volume
Papers/2011/PhysRevB_84_125411_2011.pdf, "Ming-Wei Lin, Cheng Ling, Luis A. Agapito, Nicholas K
Papers/2011/PhysRevB_84_035325_2011.pdf, "JAdam Gali, Efthimios Kaxiras, Gergely T. Zimanyi, She
```

# 2.2 Follow the stars in IMDb's list of "The Top 100 Stars for 2017"

citation\_list = parse\_for\_citations(soup)

citations\_pd = convert\_to\_pandas(citation\_list)

#### 2.2.1 Overview

In this part, your goal is to extract information from IMDb's Top 100 Stars for 2017 (https://www.imdb.com/list/ls025814950/) and perform some analysis on each star in the list. In particular we are interested to know: a) how many performers made their first movie at 17? b) how many performers started as child actors? c) who is the most proliferate actress or actor in IMDb's list of the Top 100 Stars for 2017? . These questions are addressed in more details in the Questions below.

When data is not given to us in a file, we need to fetch them using one of the following ways: - download a file from a source URL - query a database - query a web API - scrape data from the web page

Question 2 [52 pts]: Web Scraping using Beautiful Soup and exploring using Pandas

- **2.1** Download the webpage of the "Top 100 Stars for 2017" (https://www.imdb.com/list/ls025814950/) into a requests object and name it my\_page. Explain what the following attributes are:
  - my\_page.text,
  - my\_page.status\_code,
  - my\_page.content.
  - **2.2** Create a Beautiful Soup object named star\_soup using my\_page as input.
- 2.3 Write a function called parse\_stars that accepts star\_soup as its input and generates a list of dictionaries named starlist (see definition below; order of dictionaries does not matter). One of the fields of this dictionary is the url of each star's individual page, which you need to scrape and save the contents in the page field. Note that there is a ton of information about each star on these webpages.

```
name: the name of the actor/actress as it appears at the top gender: 0 or 1: translate the word 'actress' into 1 and 'actor' into '0' url: the url of the link under their name that leads to a page with details page: BS object with html text acquired by scraping the above 'url' page'
```

- **2.4** Write a function called create\_star\_table which takes starlist as an input and extracts information about each star (see function definition for the exact information to be extracted and the exact output definition). Only extract information from the first box on each star's page. If the first box is acting, consider only acting credits and the star's acting debut, if the first box is Directing, consider only directing credits and directorial debut.
- **2.5** Now that you have scraped all the info you need, it's good practice to save the last data structure you created to disk. Save the data structure to a JSON file named starinfo.json and submit this JSON file in Canvas. If you do this, if you have to restart, you won't need to redo all the requests and parsings from before.
- 2.6 We provide a JSON file called data/staff\_starinfo.json created by CS109 teaching staff for consistency, which you should use for the rest of the homework. Import the contents of this JSON file into a pandas dataframe called frame. Check the types of variables in each column and clean these variables if needed. Add a new column to your dataframe with the age of each actor when they made their first appearance, movie or TV, (name this column age\_at\_first\_movie). Check some of the values of this new column. Do you find any problems? You don't need to fix them.
- **2.7** You are now ready to answer the following intriguing questions: **2.7.1** How many performers made their first appearance (movie or TV) when he/she was 17 years old?
  - **2.7.2** How many performers started as child actors? Define child actor as a person younger than 12 years old.
- **2.8** Make a plot of the number of credits against the name of actor/actress. Who is the most prolific actress or actor in IMDb's list of the Top 100 Stars for 2017? Define **most prolific** as the performer with the most credits.

#### 2.2.2 Hints

- Create a variable that groups actors/actresses by the age of their first movie. Use pandas' .groupby to divide the dataframe into groups of performers that for example started performing as children (age < 12). The grouped variable is a GroupBy pandas object and this object has all of the information needed to then apply operations to each of the groups.
- When cleaning the data make sure the variables with which you are performing calculations are in numerical format.
- The column with the year has some values that are double, e.g. '2000-2001' and the column with age has some empty cells. You need to deal with these in a reasonable fashion before performing calculations on the data.
- You should include both movies and TV shows.

#### 2.2.3 Resources

• The requests library makes working with HTTP requests powerful and easy. For more on the requests library see http://docs.python-requests.org/

#### 2.2.4 Answers

```
In [15]: import requests
```

2.1 Download the webpage of the "Top 100 Stars for 2017 ...

```
In [201]: # your code here
    my_page = requests.get("https://www.imdb.com/list/ls025814950/")
```

your answer here \* my\_page.text is the decoded html content of the website. Requests automatically decodes the server's content. \* my\_page.status\_code is the status of the HTTP request (i.e. 202 = accepted, 400 = bad request, etc.). More information available here: https://en.wikipedia.org/wiki/List\_of\_HTTP\_status\_codes \* my\_page.content is the html content of the website provided by the server

2.2 Create a Beautiful Soup object named star\_soup giving my\_page as input.

2.3 Write a function called parse\_stars that accepts star\_soup as its input ...

```
Function
_____
parse_stars
Input
star_soup: the soup object with the scraped page
Returns
a list of dictionaries; each dictionary corresponds to a star profile and has the following da
   name: the name of the actor/actress as it appears at the top
    gender: 0 or 1: translate the word 'actress' into 1 and 'actor' into '0'
   url: the url of the link under their name that leads to a page with details
   page: BS object with 'html text acquired by scraping the above 'url' page'
Example:
{'name': Tom Hardy,
  'gender': 0,
  'url': https://www.imdb.com/name/nm0362766/?ref_=nmls_hd,
  'page': BS object with 'html text acquired by scraping the 'url' page'
}
```

```
In [252]: # your code here
          def list_of_html_profiles(soup):
              return soup.find_all('div', class_ = "lister-item-content")
          def clean text(text):
              text_to_strip = ['\n',' ',',']
              for t in text_to_strip:
                  text = text.strip(t)
              text = text.replace("\n"," ")
              return text
          def get_name(profile):
              text = profile.find('a').get_text()
              return clean_text(text)
          def get_gender(profile):
              occupation = profile.find('p', class_ = "text-muted text-small").contents[0].str
              if occupation.lower() == 'actor':
                  return 0
              elif occupation.lower() == 'actress':
                  return 1
              else:
                  return 2
          def get_url(profile):
              text = "https://www.imdb.com" + profile.find('a')['href']
              return text
          def get_page(profile):
              url = get_url(profile)
              my_page = requests.get(url)
              time.sleep(10)
              return BeautifulSoup(my_page.text, 'html.parser')
          def create_profile_dict(profile):
              profile_dict = {
                  'name': get_name(profile),
                  'gender': get_gender(profile),
                  'url': get_url(profile),
                  'page': get_page(profile)
              }
              print("scraped %s" % profile_dict['name'])
              return profile_dict
          def parse_soup(soup):
              return [create_profile_dict(p) for p in list_of_html_profiles(soup)]
```

## starlist = parse\_soup(star\_soup)

scraped Gal Gadot

scraped Tom Hardy

scraped Emilia Clarke

scraped Alexandra Daddario

scraped Bill Skarsgård

scraped Pom Klementieff

scraped Ana de Armas

scraped Dan Stevens

scraped Sofia Boutella

scraped Katherine Langford

scraped Karen Gillan

scraped Margot Robbie

scraped Felicity Jones

scraped Emma Stone

scraped Dylan Minnette

scraped Jennifer Lawrence

scraped Alicia Vikander

scraped Britt Robertson

scraped Ruby Rose

scraped Brie Larson

scraped Keanu Reeves

scraped Sophia Lillis

scraped Jessica Henwick

scraped Cara Delevingne

scraped Haley Bennett

scraped Luke Evans

scraped Teresa Palmer

scraped Tom Holland

scraped Alison Brie

scraped Robin Wright

scraped Zendaya

scraped Emma Watson

scraped Scarlett Johansson

scraped Dafne Keen

scraped Kelly Rohrbach

scraped Eiza González

scraped Laura Haddock

scraped Mary Elizabeth Winstead

scraped Taron Egerton

scraped Anya Taylor-Joy

scraped Elizabeth Debicki

scraped Katheryn Winnick

scraped Sean Young

scraped Bill Paxton

scraped Charlie Hunnam

scraped Yvonne Strahovski

scraped Jason Momoa

scraped Lily James

scraped Jodie Whittaker

scraped Ryan Gosling

scraped Adrianne Palicki

scraped Millie Bobby Brown

scraped Allison Williams

scraped Chris Pratt

scraped Katherine Waterston

scraped Tom Cruise

scraped Johnny Depp

scraped James McAvoy

scraped Travis Fimmel

scraped Charlize Theron

scraped Cole Sprouse

scraped Kaya Scodelario

scraped Abigail Breslin

scraped Daisy Ridley

scraped Emily Browning

scraped Christopher Nolan

scraped Zoe Saldana

scraped Lena Headey

scraped Hugh Jackman

scraped Kit Harington

scraped Leonardo DiCaprio

scraped Malina Weissman

scraped Finn Jones

scraped Chloë Grace Moretz

scraped Alexander Skarsgård

scraped Amy Adams

scraped Bella Thorne

scraped Rebecca Ferguson

scraped Julia Garner

scraped Joan Crawford

scraped Kate Mara

scraped Chris Pine

scraped Bryce Dallas Howard

scraped Halston Sage

scraped Kate Beckinsale

scraped Connie Nielsen

scraped Auli'i Cravalho

scraped Mädchen Amick

scraped Serinda Swan

scraped Dave Bautista

scraped Rose Leslie

scraped Annabelle Wallis

scraped Zoey Deutch

scraped Sophie Turner

```
scraped Dakota Johnson
scraped Rosamund Pike
scraped Elodie Yung
scraped Shailene Woodley
scraped Nina Dobrev
scraped Christian Navarro
  This should give you 100
In [253]: len(starlist)
Out [253]: 100
In [16]: # check your code
         # this list is large because of the html code into the `page` field
         # to get a better picture, print only the first element
         # clear/remove output before making pdf
         # print(starlist[0])
  Your output should look like this: "' {'name': 'Gal Gadot', 'gender': 1, 'url':
'https://www.imdb.com/name/nm2933757?ref_=nmls_hd', 'page':
  2.4 Write a function called create_star_table to extract information about each star ...
Function
_____
create_star_table
Input
the starlist
Returns
_____
a list of dictionaries; each dictionary corresponds to a star profile and has the following da
    star_name: the name of the actor/actress as it appears at the top
    gender: 0 or 1 (1 for 'actress' and 0 for 'actor')
    year_born : year they were born
    first_movie: title of their first movie or TV show
    year_first_movie: the year they made their first movie or TV show
    credits: number of movies or TV shows they have made in their career.
```

Example:

```
{'star_name': Tom Hardy,
     'gender': 0,
     'year_born': 1997,
     'first_movie' : 'Batman',
     'year_first_movie' : 2017,
     'credits': 24}
In [286]: starlist_copy = starlist.copy()
In [371]: def get_year(star_page):
                                  try:
                                             return star_page.find('div', {'id': 'name-born-info'}).find_all('a')[1].text
                                   except AttributeError:
                                            print('missing value')
                                            return None
                        def get_first_movie(star_page):
                                  tags = star_page.find('div', class_='filmo-category-section').find_all('a')
                                  movies = [tag.text for tag in tags if 'pisode' not in tag.text]
                                  return movies[-1]
                        def get_year_first_movie(star_page):
                                  text = star_page.find('div', class_='filmo-category-section').find_all('span', class_='film
                                  return re.sub('[^0-9-]', '', text)
                        def get_credits(star_page):
                                  try:
                                            text = star_page.find('div', id = re.compile('filmo-head-act')).text
                                            return re.sub('[^0-9]', '', text)
                                   except AttributeError:
                                            print('missing value')
                                            return None
                        def create_star_dict(old_star_dict):
                                   star_dict = {
                                             'star_name': old_star_dict['name'],
                                             'gender': old_star_dict['gender'],
                                             'year_born': get_year(old_star_dict['page']),
                                             'first_movie': get_first_movie(old_star_dict['page']),
                                             'year_first_movie': get_year_first_movie(old_star_dict['page']),
                                             'credits': get_credits(old_star_dict['page'])
                                  }
                                  return star_dict
                        def create_star_table(starlist: list) -> list:
                                   return [create_star_dict(old_star_dict) for old_star_dict in starlist]
```

```
In [372]: star_table = create_star_table(starlist)
missing value
missing value
missing value
In [17]: # check your code
         # clear/remove output before making the pdf file
         # star_table
   Your output should look like this (the order of elements is not important):
[{'name': 'Gal Gadot',
  'gender': 1,
  'year_born': '1985',
  'first_movie': 'Bubot',
  'year_first_movie': '2007',
  'credits': '25'},
 {'name': 'Tom Hardy',
  'gender': 0,
  'year_born': '1977',
  'first_movie': 'Tommaso',
  'year_first_movie': '2001',
  'credits': '55'},
   2.5 Now that you have scraped all the info you need, it's a good practice to save the last data
structure you ...
In [374]: # your code here
          import json
          with open('starinfo.json', 'w') as file:
               json.dump(star_table, file)
```

To check your JSON saving, re-open the JSON file and reload the code

2.6 Import the contents of the staff's JSON file (data/staff\_starinfo.json) into a pandas dataframe. ...

2.6 We provide a JSON file called data/staff\_starinfo.json created by CS109 teaching staff for consistency, which you should use for the rest of the homework. Import the contents of this JSON file into a pandas dataframe called frame. Check the types of variables in each column and clean these variables if needed. Add a new column to your dataframe with the age of each actor when they made their first appearance, movie or TV, (name this column age at first movie). Check some of the values of this new column. Do you find any problems? You don't need to fix them.

2007

2001

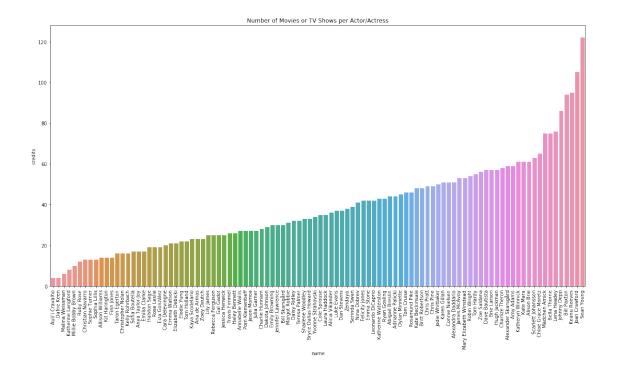
2009

2000

2002-2003

```
In [392]: # your code here
          frame = pd.read_json('./data/staff_starinfo.json')
          frame.head()
Out [392]:
             credits
                           first_movie gender
                                                               name
                                                                     year_born year_first_movie
          0
                  25
                                 Bubot
                                             1
                                                          Gal Gadot
                                                                           1985
          1
                  55
                               Tommaso
                                             0
                                                          Tom Hardy
                                                                          1977
          2
                  17
                                             1
                               Doctors
                                                      Emilia Clarke
                                                                          1986
          3
                                                Alexandra Daddario
                  51
                      All My Children
                                              1
                                                                           1986
          4
                  30
                            Järngänget
                                             0
                                                     Bill Skarsgård
                                                                           1990
In [393]: # your code here
          #check types
          print("types before cleaning:")
          print(frame.dtypes)
          #take only first year when year first movie is of format yyyy-yyyy
          frame.year_first_movie = frame.year_first_movie.apply(lambda x: x[:4])
          #cast year_first_movie to int
          frame.year_first_movie = frame.year_first_movie.astype(int)
          #check types
          print("types after cleaning:")
          print(frame.dtypes)
types before cleaning:
credits
                     int64
first_movie
                    object
                     int64
gender
name
                    object
year_born
                     int64
year_first_movie
                    object
dtype: object
types after cleaning:
credits
                     int64
first_movie
                    object
gender
                     int64
                    object
name
                     int64
year_born
```

```
year_first_movie
                      int64
dtype: object
In [397]: # your code here
          #check for missing values
          print('number of NA values: %i' %frame.isna().sum().sum())
number of NA values: 0
In [403]: # your code here
          frame['age_at_first_movie'] = frame['year_first_movie'] - frame['year_born']
          frame[frame['age_at_first_movie'] < 0]</pre>
Out [403]:
              credits
                           first_movie gender
                                                          name year_born year_first_movie
          63
                    32 Only Yesterday
                                              1 Daisy Ridley
                                                                      1992
   your answer here
   Daisy Ridley's first movie was apparently released before she was born.
   2.7 You are now ready to answer the following intriguing questions:
   2.7.1 How many performers made their first movie at 17?
In [409]: # your code here
          print("%i performers made their first movie at 17" % frame.groupby('age_at_first_mov
8 performers made their first movie at 17
   Your output should look like this: 8 performers made their first movie at 17
   2.7.2 How many performers started as child actors? Define child actor as a person less than
12 years old.
In [414]: # your code here
          print("%i performers started as child actors" % frame[frame.age_at_first_movie < 12]</pre>
20 performers started as child actors
   2.8 Make a plot of the number of credits versus the name of actor/actress.
In [437]: # your code here
          frame = frame.sort_values('credits')
          plt.subplots(figsize=(20,10))
          ax = sns.barplot(x = frame.name, y = frame.credits)
          ax.set_title('Number of Movies or TV Shows per Actor/Actress')
          ax.set_xticklabels(frame.name, rotation=90)
          plt.figure(figsize=(40,10))
Out[437]: <Figure size 2880x720 with 0 Axes>
```



<Figure size 2880x720 with 0 Axes>

The most prolific actor is Sean Young

## 2.3 Going the Extra Mile

Be sure to complete problems 1 and 2 before tackling this problem...it is worth only 8 points.

Question 3 [8 pts]: Parsing using Regular Expressions (regex)

Even though scraping HTML with regex is sometimes considered bad practice, you are to use python's **regular expressions** to answer this problem. Regular expressions are useful to parse strings, text, tweets, etc. in general (for example, you may encounter a non-standard format for dates at some point). Do not use BeautifulSoup to answer this problem.

- 3.1 Write a function called get\_pubs that takes an .html filename as an input and returns a string containing the HTML page in this file (see definition below). Call this function using data/publist\_super\_clean.html as input and name the returned string prof\_pubs.
- **3.2** Calculate how many times the author named 'C.M. Friend' appears in the list of publications.
  - **3.3** Find all unique journals and copy them in a variable named journals.
- **3.4** Create a list named pub\_authors whose elements are strings containing the authors' names for each paper.

#### 2.3.1 Hints

- Look for patterns in the HTML tags that reveal where each piece of information such as the title of the paper, the names of the authors, the journal name, is stored. For example, you might notice that the journal name(s) is contained between the <I> HTML tag.
- Learning about your domain is always a good idea: you want to check the names to make sure that they belong to actual journals. Thus, while journal name(s) is contained between the <I> HTML tag, please note that all strings found between <I> tags may not be journal names.
- Each publication has multiple authors.
- C.M. Friend also shows up as Cynthia M. Friend in the file. Count just C. M. Friend.
- There is a comma at the end of the string of authors. You can choose to keep it in the string or remove it and put it back when you write the string as a BibTex entry.
- You want to remove duplicates from the list of journals. Duplicates may also occur due to misspellings or spaces, such as: Nano Lett., and NanoLett. You can assume that any journals with the same initials (e.g., NL for NanoLett.) are the same journal.

#### 2.3.2 Resources

- **Regular expressions:** a) https://docs.python.org/3.3/library/re.html, b) https://regexone.com, and c) https://docs.python.org/3/howto/regex.html.
- \*\* HTML:\*\* if you are not familiar with HTML see https://www.w3schools.com/html/ or one of the many tutorials on the internet.
- \*\* Document Object Model (DOM):\*\* for more on this programming interface for HTML and XML documents see https://www.w3schools.com/js/js\_htmldom.asp.

## 2.3.3 Answers

\*\* 3.1 Write a function called get\_pubs that takes an .html filename as an input and returns a string \*\*

You should see an HTML page that looks like this (colors are not important) "'html

"Approaching the intrinsic band gap in suspended high-mobility graphene nanoribbons" Ming-Wei Lin, Cheng Ling, Luis A. Agapito, Nicholas Kioussis, Yiyang Zhang, Mark Ming-Cheng Cheng, PHYSICAL REVIEW B 84, 125411 (2011)

"Effect of symmetry breaking on the optical absorption of semiconductor nanoparticles" JAdam Gali, Efthimios Kaxiras, Gergely T. Zimanyi, Sheng Meng, PHYSICAL REVIEW B 84, 035325 (2011)

"Influence of CH2 content and network defects on the elastic properties of organosilicate glasses" Jan M. Knaup, Han Li, Joost J. Vlassak, and Efthimios Kaxiras, PHYSICAL REVIEW B 83, 054204 (2011)

. . .

### 3.2 Calculate how many times the author ...

```
In [524]: # your code here
          print("C.M. Friend appears %i times"%prof_pubs.count("C.M. Friend"))
C.M. Friend appears 5 times
  3.3 Find all unique journals and copy ...
In [525]: # your code here
          journals_with_tags = set(re.findall("<I>.*</I>",prof_pubs))
          journals = [name[3:-5] for name in journals_with_tags]
          journals.sort()
          journals.remove('NanoLett.')
          journals.remove('New J. Phys.')
In [526]: journals
Out[526]: ['2010 ACM/IEEE International Conference for High Performance',
           'ACSNano.',
           'Ab initi',
           'Acta Mater.',
           'Catal. Sci. Technol.',
           'Chem. Eur. J.',
           'Comp. Phys. Comm.',
           'Concurrency Computat.: Pract. Exper.',
           'Energy & Environmental Sci.',
           'Int. J. Cardiovasc. Imaging',
           'J. Chem. Phys.',
           'J. Chem. Theory Comput.',
           'J. Phys. Chem. B',
           'J. Phys. Chem. C',
           'J. Phys. Chem. Lett.',
```

'J. Stat. Mech: Th. and Exper.',

'Langmuir',

```
'Molec. Phys.',
'Nano Lett.',
'New Journal of Physics',
'PHYSICAL REVIEW B',
'Phil. Trans. R. Soc. A',
'Phys. Rev. B',
'Phys. Rev. E - Rap. Comm.',
'Phys. Rev. Lett.',
'Sci. Model. Simul.',
'Sol. St. Comm.',
'Top. Catal.']
```

Your output should look like this (no duplicates): {'2010 ACM/IEEE International Conference for High Performance', 'ACSNano.', 'Ab initio', 'Acta Mater.', 'Catal. Sci. Technol.', 'Chem. Eur. J.', 'Comp. Phys. Comm.', 'Concurrency Computat.: Pract. Exper.', 'Energy & Environmental Sci.', 'Int. J. Cardiovasc. Imaging', 'J. Chem. Phys.', 'J. Chem. Theory Comput.', 'J. Phys. Chem. B', 'J. Phys. Chem. C', 'J. Phys. Chem. Lett.', 'J. Stat. Mech: Th. and Exper.', 'Langmuir', 'Molec. Phys.', 'Nano Lett.', 'New Journal of Physics', 'PHYSICAL REVIEW B', 'Phil. Trans. R. Soc. A', 'Phys. Rev. E - Rap. Comm.', 'Phys. Rev. Lett.', 'Sci. Model. Simul.', 'Sol. St. Comm.', 'Top. Catal.'}

## 3.4 Create a list named pub\_authors...

L.A. Agapito, N. Kioussis and E. Kaxiras

Ming-Wei Lin, Cheng Ling, Luis A. Agapito, Nicholas Kioussis, Yiyang Zhang, Mark Ming-Cheng Cheng Chen JAdam Gali, Efthimios Kaxiras, Gergely T. Zimanyi, Sheng Meng Jan M. Knaup, Han Li, Joost J. Vlassak, and Efthimios Kaxiras Martin Heiss, Sonia Conesa-Boj, Jun Ren, Hsiang-Han Tseng, Adam Gali Simone Melchionna, Efthimios Kaxiras, Massimo Bernaschi and Sauro Succi J R Maze, A Gali, E Togan, Y Chu, A Trifonov Kejie Zhao, Wei L. Wang, John Gregoire, Matt Pharr, Zhigang Suo Masataka Katono, Takeru Bessho, Sheng Meng, Robin Humphry-Baker, Guido Rothenberger Thomas D. Kuhne, Tod A. Pascal, Efthimios Kaxiras, and Yousung Jung Sheng Meng, Efthimios Kaxiras, Md. K. Nazeeruddin, and Michael Gratzel Bingjun Xu, Jan Haubrich, Thomas A. Baker, Efthimios Kaxiras, and Cynthia M. Friend Jun Ren, Sheng Meng, Yi-Lin Wang, Xu-Cun Ma, Qi-Kun Xue, Efthimios Kaxiras Jan Haubrich, Efthimios Kaxiras, and Cynthia M. Friend Thomas A. Baker, Bingjun Xu, Stephen C. Jensen, Cynthia M. Friend and Efthimios Kaxiras Youdong Mao, Wei L. Wang, Dongguang Wei, Efthimios Kaxiras, and Joseph G. Sodroski H. Li, J.M. Knaup, E. Kaxiras and J.J. Vlassak W.L. Wang and E. Kaxiras

- A. Peters, S. Melchionna, E. Kaxiras, J. Latt, J. Sircar, S. Succi
- J. Ren, E. Kaxiras and S. Meng
- T.A. Baker, E. Kaxiras and C.M. Friend
- H.P. Chen, R.K. Kalia, E. Kaxiras, G. Lu, A. Nakano, K. Nomura
- S. Meng and E. Kaxiras
- C.L. Chang, S.K.R.S. Sankaranarayanan, D. Ruzmetov, M.H. Engelhard, E. Kaxiras and S. Ramanath
- T.A. Baker, C.M. Friend and E. Kaxiras
- S. Melchionna, M. Bernaschi, S. Succi, E. Kaxiras, F.J. Rybicki, D. Mitsouras, A.U. Coskun and
- M. Bernaschi, M. Fatica, S. Melchionna, S. Succi and E. Kaxiras
- E. Manousakis, J. Ren, S. Meng and E. Kaxiras
- A. Gali, E. Janzen, P. Deak, G. Kresse and E. Kaxiras
- S.K.R.S. Sankaranarayanan, E. Kaxiras and S. Ramanathan
- M. Bernaschi, S. Melchionna, S. Succi, M. Fyta, E. Kaxiras
- T.A. Baker, B.J. Xu, X.Y. Liu, E. Kaxiras and C.M. Friend
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