Utrecht University
Exam Structure of Matter
Thursday, March 7th, 2019
Time: 9:00 - 12:00

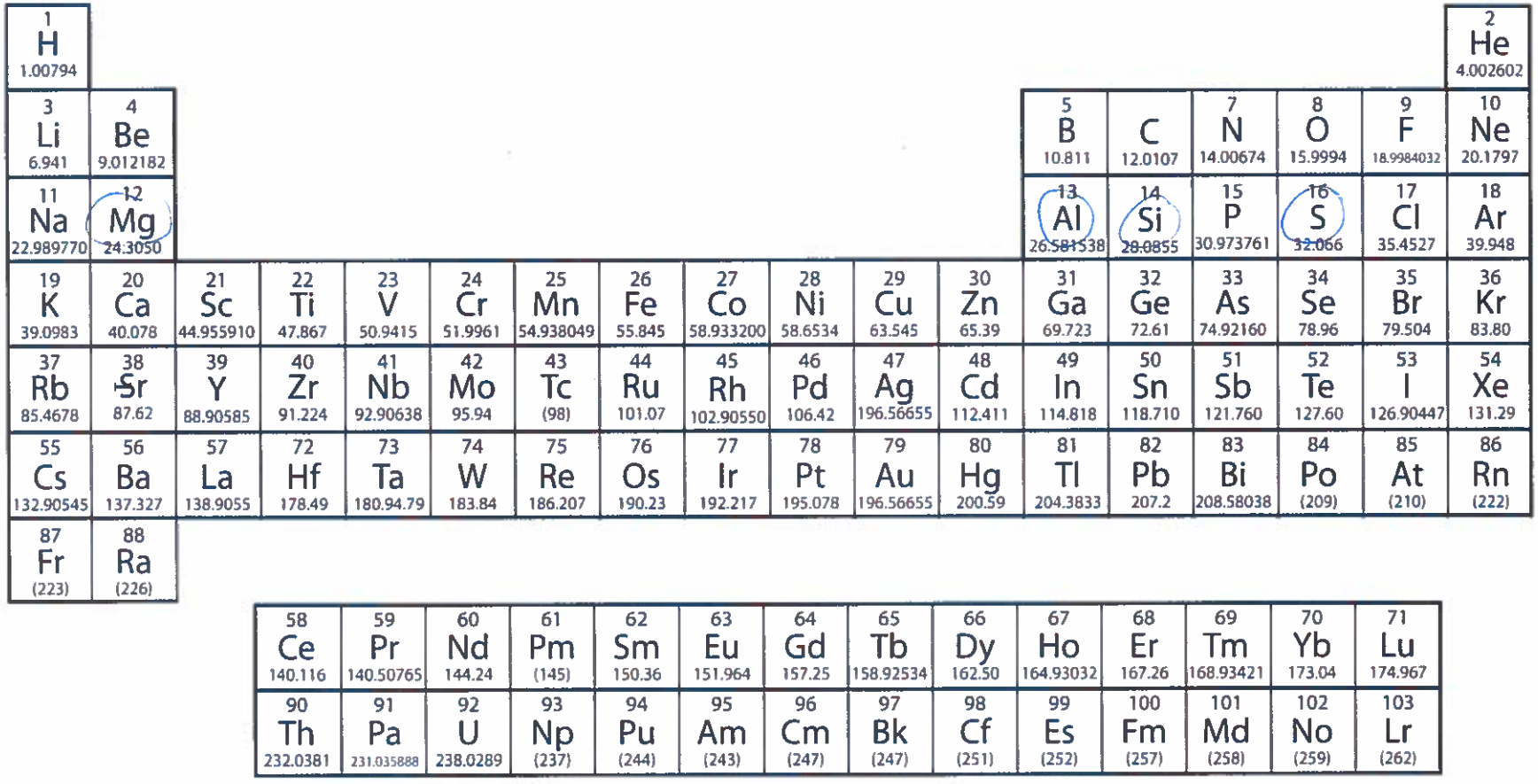
Name and student number: _____

Good luck!

Write your answers to questions 1, 2, and 3 on one sheet, and the answers to question 4 on a second sheet.

- Please pay attention to your hand-writing. If we cannot read your answers, we cannot award points.
- In your answers, do not immediately start with equations. Also draw conclusions from the calculations you have done.
- Calculators, graphical or otherwise, are not allowed.
- Please note that you can earn a maximum of 61 points.
- Not each question is worth the same number of points.
- Questions have been ordered by subject, not by difficulty. Suggestion: save the most difficult/time consuming questions for last.
- The following relations might be helpful:

$$\cos(2a) = 2\cos^2 a - 1$$
$$\cos(a+b) = \cos(a)\cos(b) - \sin(a)\sin(b)$$
$$\cos(a-b) = \cos(a)\cos(b) + \sin(a)\sin(b)$$
$$e^{ik} + e^{-ik} = 2\cos(k)$$
$$\int_{-\infty}^{\infty} f(x)\delta(x-x_0)\,dx = f(x_0)$$


1 H 1.00794
2 He 4.002602
3 Li 6.941
4 Be 9.012182
5 B 10.811
C 12.0107
7 N 14.00674
8 O 15.9994
9 F 18.9984032
10 Ne 20.1797
11 Na 22.989770
12 Mg 24.3050
13 Al 26.581538
14 Si 28.0855
15 P 30.973761
16 S 32.066
17 Cl 35.4527
18 Ar 39.948
19 K 39.0983
20 Ca 40.078
21 Sc 44.955910
22 Ti 47.867
23 V 50.9415
24 Cr 51.9961
25 Mn 54.938049
26 Fe 55.845
27 Co 58.933200
28 Ni 58.6534
29 Cu 63.545
30 Zn 65.39
31 Ga 69.723
32 Ge 72.61
33 As 74.92160
34 Se 78.96
35 Br 79.504
36 Kr 83.80
37 Rb 85.4678
38 Sr 87.62
39 Y 88.90585
40 Zr 91.224
41 Nb 92.90638
42 Mo 95.94
43 Tc (98)
44 Ru 101.07
45 Rh 102.90550
46 Pd 106.42
47 Ag 196.56655
48 Cd 112.411
49 In 114.818
50 Sn 118.710
51 Sb 121.760
52 Te 127.60
53 I 126.90447
54 Xe 131.29
55 Cs 132.90545
56 Ba 137.327
57 La 138.9055
72 Hf 178.49
73 Ta 180.94.79
74 W 183.84
75 Re 186.207
76 Os 190.23
77 Ir 192.217
78 Pt 195.078
79 Au 196.56655
80 Hg 200.59
81 Tl 204.3833
82 Pb 207.2
83 Bi 208.58038
84 Po (209)
85 At (210)
86 Rn (222)
87 Fr (223)
88 Ra (226)
58 Ce 140.116
59 Pr 140.50765
60 Nd 144.24
61 Pm (145)
62 Sm 150.36
63 Eu 151.964
64 Gd 157.25
65 Tb 158.92534
66 Dy 162.50
67 Ho 164.93032
68 Er 167.26
69 Tm 168.93421
70 Yb 173.04
71 Lu 174.967
90 Th 232.0381
91 Pa 231.035888
92 U 238.0289
93 Np (237)
94 Pu (244)
95 Am (243)
96 Cm (247)
97 Bk (247)
98 Cf (251)
99 Es (252)
100 Fm (257)
101 Md (258)
102 No (259)
103 Lr (262)

Question 1: **Atomic Physics** ..... *7 points*

(a) (1 point) Give the electron configuration of Se ($Z = 34$)

(b) (4 points) In 1974, an element with 106 protons was synthesized. In 1997, this element was named Seaborgium (symbol: Sg), after the American physicist Glenn T. Seaborg. Its most stable isotope has a half-life of approximately 14 minutes, which is sufficiently long to study basic chemical properties. What do you expect for the chemical properties of this element?

(c) (1 point) Electronegativity is a property of atoms that describes the tendency of an atom to attract electron density towards itself. An atom's electronegativity is affected by both its atomic number and the distance at which its valence electrons reside from the nucleus. Why is the electronegativity value of most noble gases zero?

(d) (1 point) Arrange these atoms in order of decreasing effective nuclear charge by the valence electrons: Si, Al, Mg, S

Question 2: **Molecular Physics** ..... *10 points*

(a) (1 point) What is the order of magnitude of the energy associated with a covalent bond?

(b) (1 point) What is the order of magnitude of the length associated with a covalent bond?

(c) (2 points) Is orbital hybridization required to describe the electronic structure of molecules?

(d) (3 points) The allene molecule $CH_2{=}C{=}CH_2$ is known to have a linear geometry for the three carbon atoms. Rationalize this on the basis of hybridization of atomic orbitals of the central C atom. Include the names of the types of covalent bonds that are formed in your answer.

(e) (3 points) Why does the He_2 molecule not exist?

Question 3: **Soft Matter** ..... *9 points*

(a) (3 points) The size of a polymer chain can be defined in various ways. In class, the (mean-squared) end-to-end distance was used. In addition, one could use the so-called radius of gyration of the macromolecule, R_g, see Figure 1.

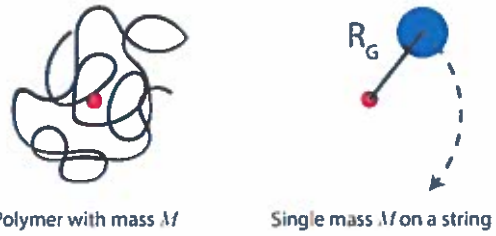


Figure 1: Left: model of a polymer with mass M. The center of mass is indicated by the red dot. The polymer can rotate. Conceptually, the rotating polymer can be replaced by a single particle (blue) on a string swinging around. The polymer and conceptual system have the same moment of inertia. The radius of gyration is defined as the length of the string connecting the particle to the center of mass.

For a polymer chain of N monomer units, the radius of gyration is defined as

$$R_G^2 = \frac{1}{N+1}\sum_{i=0}^{N}\langle(\mathbf{R_i}-\mathbf{R_{CM}})^2\rangle$$
$$= \frac{1}{N+1}\sum_{i=0}^{N}\left\langle\left(\mathbf{R_i}-\frac{1}{N+1}\sum_{j=0}^{N}\mathbf{R_j}\right)^2\right\rangle$$

with $\mathbf{R_i}$ the position of bead or vertex i of the polymer chain and $\mathbf{R_{CM}}$ is the position of the center of mass of the polymer chain. Show that the following expression holds

$$R_G^2 = \frac{1}{2(N+1)^2}\sum_{i=0}^{N}\sum_{j=0}^{N}\langle(\mathbf{R_i}-\mathbf{R_j})^2\rangle \tag{1}$$

(b) (4 points) The expression found above can be rewritten as

$$R_G^2 = \frac{1}{(N+1)^2}\sum_{i=1}^{N}\sum_{j=0}^{i-1} b^2(i-j) \tag{2}$$

where b is the length of a monomer in the polymer chain, and i, j indices. Show that the radius of gyration of the freely jointed chain is given by

$$R_G^2 \approx \frac{b^2 N}{6} \tag{3}$$

Hint: Realize that for a polymer N is (very) large.

(c) (2 points) How does the radius of gyration compare to the end-to-end distance of a freely jointed chain?

Question 4: **Condensed Matter Physics** ..... *35 points*

(a) (2 points) Hexagonal Boron Nitride (h-BN) has a structure similar to graphene, see Figure 2 below. The 'only' difference is that the material contains equal amounts of N ($Z = 7$) and B ($Z = 5$) instead of C ($Z = 6$). Indicate the Wigner-Seitz cell of h-BN **AND** a primitive unit cell.

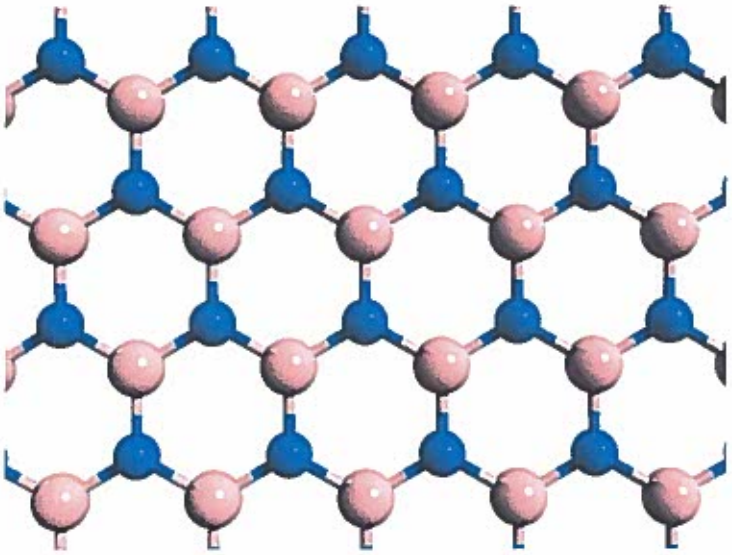


Figure 2: Crystal of hexagonal boron nitride. N and B atoms are indicated in blue and mauve, respectively.

(b) (5 points) Assume that the lattice vectors are given by:

$$\mathbf{a}_1 = \left(\frac{3a}{2}, \frac{\sqrt{3}a}{2}\right), \mathbf{a}_2 = \left(\frac{3a}{2}, \frac{-\sqrt{3}a}{2}\right) \tag{4}$$

Determine the reciprocal space unit cell of h-BN.

(c) (19 points) Show that a nearest-neighbor tight-binding calculation, only taking into account $2p_z$ orbitals, results in the following dispersion relation for h-BN.

$$E(\boldsymbol{k}) = \alpha_{av} \pm \sqrt{\alpha_{av}^2 - \alpha_B \alpha_N + \beta^2 f(\boldsymbol{k})} \tag{5}$$

with $\alpha_{av} = \frac{\alpha_B + \alpha_N}{2}$ and $f(\boldsymbol{k}) = 3 + 4\cos\left(\frac{3a}{2}k_x\right)\cos\left(\frac{\sqrt{3}a}{2}k_y\right) + 2\cos\left(\sqrt{3}ak_y\right)$.

(d) (2 points) What do α_i and β correspond to physically?

(e) (7 points) Assume that α_B and α_N *differ* by an amount x eV. Use equation 5 to show that h-BN is either a conductor, insulator or 'graphene-like' material.